



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 2B5L / pdb\_00002b5l  
Title : Crystal Structure of DDB1 In Complex with Simian Virus 5 V Protein  
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Deposited on : 2005-09-28  
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

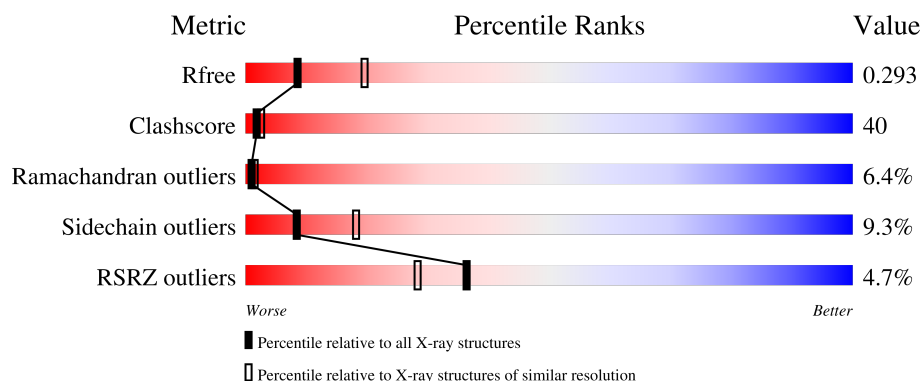
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1407 (2.88-2.84)                                      |
| Clashscore            | 190562                      | 1446 (2.88-2.84)                                      |
| Ramachandran outliers | 187476                      | 1406 (2.88-2.84)                                      |
| Sidechain outliers    | 187428                      | 1407 (2.88-2.84)                                      |
| RSRZ outliers         | 180081                      | 1408 (2.88-2.84)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 1140   | <div> <div>2%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>9%</div> <div>..</div> </div> </div>                 |
| 1   | B     | 1140   | <div> <div>4%</div> <div> <div></div> <div>38%</div> <div>47%</div> <div>12%</div> <div>..</div> </div> </div>                |
| 2   | C     | 222    | <div> <div>9%</div> <div> <div></div> <div>27%</div> <div>36%</div> <div>13%</div> <div>.</div> <div>22%</div> </div> </div>  |
| 2   | D     | 222    | <div> <div>14%</div> <div> <div></div> <div>23%</div> <div>36%</div> <div>16%</div> <div>.</div> <div>21%</div> </div> </div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20399 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called damage-specific DNA binding protein 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1132     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8860  | 5610 | 1493 | 1708 | 49 |         |         |       |
| 1   | B     | 1134     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8876  | 5619 | 1495 | 1713 | 49 |         |         |       |

- Molecule 2 is a protein called Nonstructural protein V.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | C     | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 826 | 229 | 261 | 8 |         |         |       |
| 2   | D     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1335  | 834 | 233 | 260 | 8 |         |         |       |

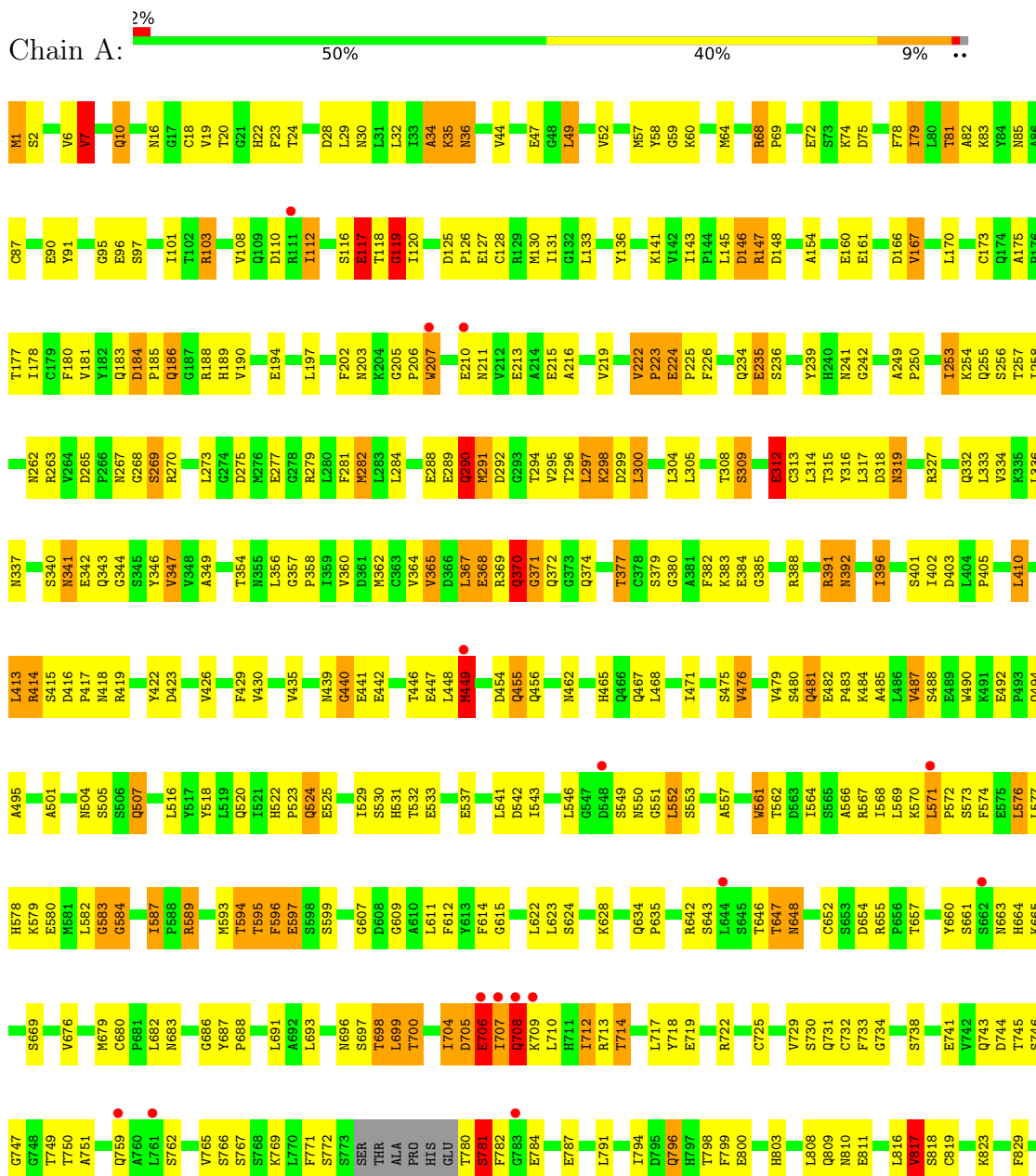
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

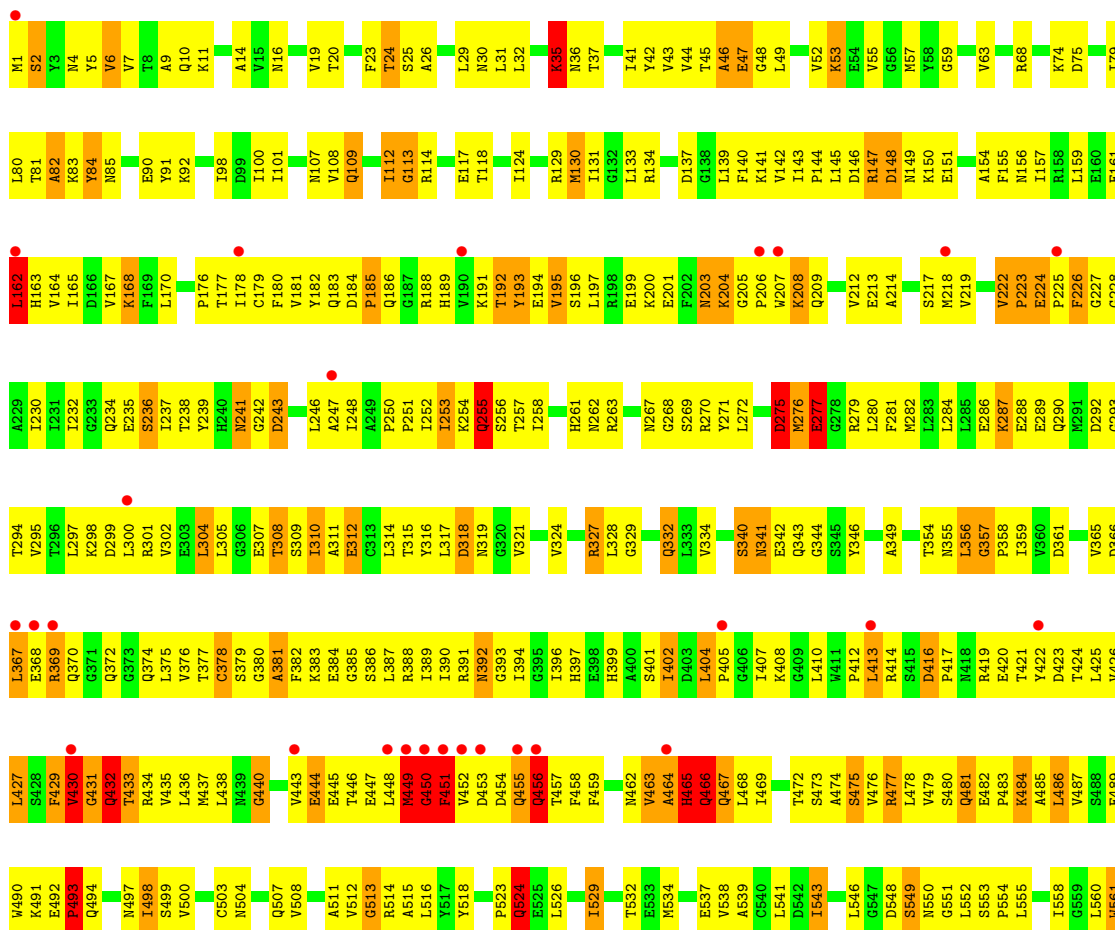
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | C     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

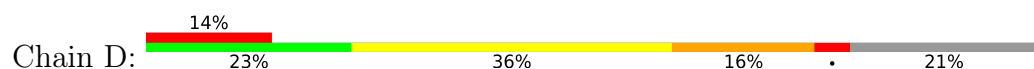
### 3 Residue-property plots

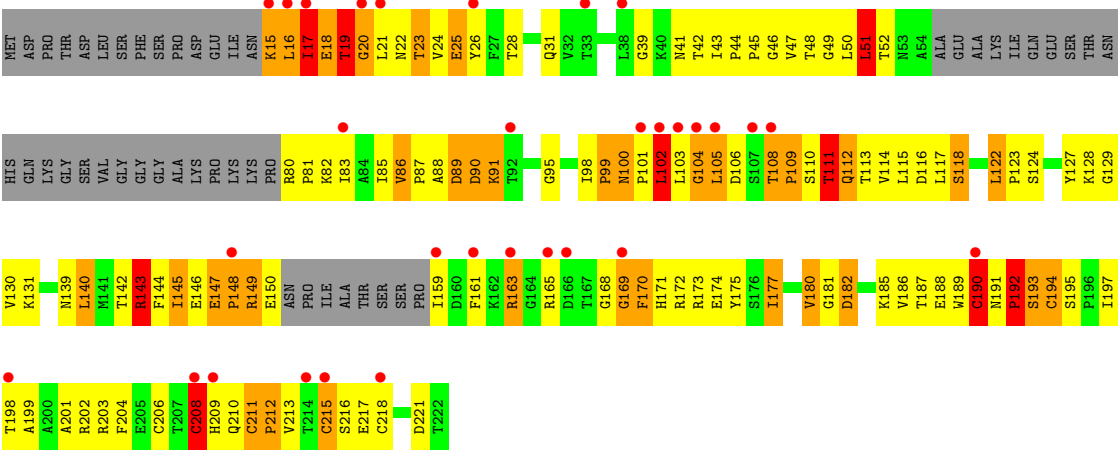
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: damage-specific DNA binding protein 1









## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 62.76Å 240.79Å 117.18Å<br>90.00° 101.79° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 47.80 – 2.85<br>47.80 – 2.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (47.80-2.85)<br>95.7 (47.80-2.85)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.84 (at 2.65Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.229 , 0.299<br>0.226 , 0.293                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3805 reflections (4.13%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.604                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 64.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 20399                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 64.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.57         | 5/9022 (0.1%)   | 1.13        | 81/12219 (0.7%)  |
| 1   | B     | 0.60         | 14/9039 (0.2%)  | 1.32        | 118/12244 (1.0%) |
| 2   | C     | 0.79         | 8/1351 (0.6%)   | 1.42        | 27/1832 (1.5%)   |
| 2   | D     | 1.08         | 4/1361 (0.3%)   | 1.63        | 32/1843 (1.7%)   |
| All | All   | 0.64         | 31/20773 (0.1%) | 1.27        | 258/28138 (0.9%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 1                   | 1                   |
| 2   | D     | 0                   | 1                   |
| All | All   | 1                   | 2                   |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2   | D     | 189 | TRP  | C-N   | -25.44 | 0.99        | 1.33     |
| 2   | D     | 190 | CYS  | C-N   | 17.91  | 1.59        | 1.33     |
| 1   | B     | 431 | GLY  | N-CA  | -12.68 | 1.35        | 1.45     |
| 1   | B     | 430 | VAL  | C-N   | -9.31  | 1.25        | 1.33     |
| 1   | B     | 455 | GLN  | N-CA  | -8.16  | 1.35        | 1.46     |
| 1   | A     | 706 | GLU  | C-N   | -8.13  | 1.26        | 1.33     |
| 2   | C     | 37  | SER  | CA-C  | -7.72  | 1.45        | 1.53     |
| 1   | B     | 429 | PHE  | CA-C  | -7.55  | 1.44        | 1.53     |
| 1   | B     | 749 | THR  | C-N   | -7.36  | 1.23        | 1.33     |
| 1   | B     | 748 | GLY  | N-CA  | -7.27  | 1.34        | 1.45     |
| 1   | B     | 430 | VAL  | N-CA  | -7.01  | 1.37        | 1.46     |
| 2   | C     | 190 | CYS  | C-N   | 7.00   | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 750 | THR  | N-CA   | -6.29 | 1.38        | 1.46     |
| 2   | D     | 170 | PHE  | N-CA   | -6.28 | 1.37        | 1.45     |
| 1   | A     | 597 | GLU  | N-CA   | -6.19 | 1.40        | 1.46     |
| 1   | A     | 707 | ILE  | N-CA   | -6.03 | 1.39        | 1.46     |
| 2   | C     | 36  | SER  | C-N    | -5.80 | 1.26        | 1.34     |
| 1   | A     | 596 | PHE  | C-N    | -5.60 | 1.27        | 1.33     |
| 1   | A     | 899 | VAL  | CA-CB  | 5.47  | 1.60        | 1.54     |
| 1   | B     | 464 | ALA  | N-CA   | 5.47  | 1.53        | 1.46     |
| 2   | C     | 36  | SER  | N-CA   | -5.46 | 1.39        | 1.46     |
| 1   | B     | 429 | PHE  | CA-CB  | -5.46 | 1.48        | 1.53     |
| 2   | C     | 38  | LEU  | N-CA   | -5.40 | 1.39        | 1.46     |
| 1   | B     | 192 | THR  | C-N    | -5.35 | 1.26        | 1.33     |
| 1   | B     | 450 | GLY  | C-N    | -5.32 | 1.26        | 1.33     |
| 1   | B     | 450 | GLY  | CA-C   | -5.24 | 1.44        | 1.51     |
| 2   | C     | 33  | THR  | CB-OG1 | 5.21  | 1.52        | 1.43     |
| 2   | C     | 53  | ASN  | N-CA   | -5.18 | 1.39        | 1.46     |
| 2   | D     | 169 | GLY  | C-N    | -5.17 | 1.26        | 1.33     |
| 2   | C     | 37  | SER  | C-N    | -5.04 | 1.26        | 1.33     |
| 1   | B     | 366 | ASP  | CA-C   | -5.01 | 1.47        | 1.53     |

All (258) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 431 | GLY  | N-CA-C     | -42.26 | 71.75       | 110.21   |
| 1   | B     | 749 | THR  | N-CA-C     | -31.14 | 58.10       | 108.55   |
| 1   | B     | 35  | LYS  | CB-CA-C    | 18.23  | 146.70      | 110.42   |
| 1   | B     | 980 | ASP  | N-CA-C     | -17.33 | 78.02       | 108.69   |
| 1   | B     | 884 | ILE  | CB-CA-C    | 16.86  | 138.94      | 111.29   |
| 1   | B     | 942 | PHE  | CB-CA-C    | -16.67 | 85.50       | 111.17   |
| 2   | D     | 15  | LYS  | N-CA-C     | -16.37 | 65.16       | 111.00   |
| 1   | B     | 749 | THR  | N-CA-CB    | 14.95  | 137.44      | 110.99   |
| 2   | D     | 16  | LEU  | N-CA-CB    | -14.10 | 89.87       | 110.17   |
| 1   | A     | 202 | PHE  | CB-CA-C    | -13.28 | 89.36       | 110.74   |
| 2   | D     | 17  | ILE  | N-CA-CB    | -13.01 | 95.51       | 111.90   |
| 2   | D     | 189 | TRP  | CA-C-N     | 12.47  | 140.58      | 122.99   |
| 2   | D     | 189 | TRP  | C-N-CA     | 12.47  | 140.58      | 122.99   |
| 1   | B     | 2   | SER  | N-CA-CB    | -12.07 | 90.44       | 111.08   |
| 1   | B     | 980 | ASP  | CB-CA-C    | -11.54 | 89.46       | 109.65   |
| 1   | B     | 885 | ASN  | N-CA-C     | -11.16 | 94.72       | 111.34   |
| 1   | B     | 748 | GLY  | N-CA-C     | 11.04  | 139.33      | 113.18   |
| 1   | A     | 708 | GLN  | OE1-CD-NE2 | -10.95 | 111.65      | 122.60   |
| 2   | D     | 111 | THR  | N-CA-C     | -10.92 | 90.86       | 108.55   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 431 | GLY  | O-C-N      | 10.80  | 127.90      | 121.85   |
| 2   | D     | 16  | LEU  | CB-CA-C    | -10.79 | 89.69       | 109.54   |
| 1   | B     | 430 | VAL  | CA-C-N     | -10.74 | 107.85      | 123.95   |
| 1   | B     | 430 | VAL  | C-N-CA     | -10.74 | 107.85      | 123.95   |
| 2   | D     | 143 | ARG  | CB-CA-C    | -10.34 | 89.84       | 110.42   |
| 1   | B     | 185 | PRO  | CA-N-CD    | -10.21 | 97.70       | 112.00   |
| 2   | D     | 112 | GLN  | OE1-CD-NE2 | -10.21 | 112.39      | 122.60   |
| 1   | B     | 117 | GLU  | N-CA-C     | 10.16  | 124.94      | 112.54   |
| 1   | B     | 186 | GLN  | OE1-CD-NE2 | -10.15 | 112.44      | 122.60   |
| 1   | B     | 561 | TRP  | N-CA-C     | 10.14  | 128.82      | 113.61   |
| 1   | B     | 743 | GLN  | OE1-CD-NE2 | -10.03 | 112.57      | 122.60   |
| 2   | C     | 52  | THR  | CA-C-N     | -9.95  | 105.15      | 122.07   |
| 2   | C     | 52  | THR  | C-N-CA     | -9.95  | 105.15      | 122.07   |
| 1   | B     | 467 | GLN  | OE1-CD-NE2 | -9.92  | 112.68      | 122.60   |
| 2   | D     | 192 | PRO  | CA-N-CD    | -9.90  | 98.15       | 112.00   |
| 1   | B     | 370 | GLN  | OE1-CD-NE2 | -9.88  | 112.72      | 122.60   |
| 2   | C     | 36  | SER  | N-CA-C     | -9.85  | 94.42       | 109.79   |
| 1   | A     | 290 | GLN  | OE1-CD-NE2 | -9.82  | 112.78      | 122.60   |
| 1   | B     | 456 | GLN  | OE1-CD-NE2 | -9.77  | 112.83      | 122.60   |
| 1   | B     | 455 | GLN  | OE1-CD-NE2 | -9.74  | 112.86      | 122.60   |
| 1   | B     | 981 | SER  | N-CA-CB    | -9.64  | 93.67       | 110.44   |
| 1   | B     | 466 | GLN  | OE1-CD-NE2 | -9.61  | 112.99      | 122.60   |
| 1   | A     | 370 | GLN  | OE1-CD-NE2 | -9.55  | 113.05      | 122.60   |
| 2   | D     | 181 | GLY  | N-CA-C     | -9.33  | 103.09      | 111.67   |
| 2   | D     | 189 | TRP  | O-C-N      | -9.17  | 114.12      | 123.29   |
| 2   | C     | 86  | VAL  | N-CA-C     | 9.15   | 116.70      | 109.19   |
| 1   | A     | 909 | ILE  | N-CA-C     | -9.03  | 103.06      | 111.45   |
| 1   | B     | 36  | ASN  | N-CA-CB    | -9.03  | 95.24       | 110.49   |
| 1   | B     | 451 | PHE  | CB-CA-C    | -8.97  | 92.56       | 110.42   |
| 1   | B     | 455 | GLN  | N-CA-C     | -8.94  | 91.77       | 110.80   |
| 1   | B     | 1   | MET  | CB-CA-C    | 8.93   | 127.06      | 110.10   |
| 2   | D     | 19  | THR  | CA-C-N     | -8.90  | 103.96      | 121.41   |
| 2   | D     | 19  | THR  | C-N-CA     | -8.90  | 103.96      | 121.41   |
| 1   | A     | 609 | GLY  | N-CA-C     | -8.90  | 102.89      | 115.43   |
| 1   | A     | 290 | GLN  | CB-CA-C    | 8.89   | 128.12      | 110.42   |
| 2   | C     | 37  | SER  | N-CA-C     | -8.86  | 92.14       | 107.20   |
| 1   | B     | 432 | GLN  | OE1-CD-NE2 | -8.86  | 113.75      | 122.60   |
| 2   | D     | 15  | LYS  | CB-CA-C    | 8.83   | 126.87      | 110.10   |
| 1   | B     | 193 | TYR  | N-CA-C     | -8.76  | 95.23       | 108.46   |
| 1   | A     | 712 | ILE  | N-CA-C     | 8.49   | 118.91      | 106.85   |
| 1   | B     | 561 | TRP  | CB-CA-C    | -8.48  | 95.23       | 109.99   |
| 2   | C     | 37  | SER  | CB-CA-C    | -8.41  | 101.00      | 111.43   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | D     | 16   | LEU  | N-CA-C    | -8.41 | 98.64       | 110.50   |
| 1   | B     | 885  | ASN  | N-CA-CB   | -8.36 | 93.81       | 111.21   |
| 1   | B     | 429  | PHE  | N-CA-C    | -8.23 | 91.63       | 108.18   |
| 1   | A     | 925  | ASP  | CA-CB-CG  | 8.21  | 120.81      | 112.60   |
| 1   | B     | 1107 | GLU  | N-CA-C    | -8.16 | 102.39      | 111.28   |
| 2   | C     | 211  | CYS  | CA-C-N    | 8.10  | 129.18      | 120.11   |
| 2   | C     | 211  | CYS  | C-N-CA    | 8.10  | 129.18      | 120.11   |
| 1   | A     | 312  | GLU  | N-CA-C    | -8.04 | 102.23      | 112.93   |
| 1   | A     | 1061 | VAL  | N-CA-C    | 8.01  | 118.70      | 111.81   |
| 1   | B     | 185  | PRO  | N-CA-C    | 7.99  | 128.92      | 112.47   |
| 1   | A     | 561  | TRP  | N-CA-C    | 7.82  | 119.58      | 111.14   |
| 1   | B     | 750  | THR  | CB-CA-C   | -7.72 | 95.06       | 110.42   |
| 1   | B     | 431  | GLY  | CA-C-N    | 7.70  | 136.25      | 121.54   |
| 1   | B     | 431  | GLY  | C-N-CA    | 7.70  | 136.25      | 121.54   |
| 1   | B     | 277  | GLU  | N-CA-C    | -7.69 | 103.72      | 113.72   |
| 1   | B     | 35   | LYS  | N-CA-C    | -7.66 | 94.47       | 110.80   |
| 2   | C     | 182  | ASP  | N-CA-C    | -7.57 | 104.55      | 114.31   |
| 2   | D     | 20   | GLY  | N-CA-C    | 7.50  | 130.95      | 113.18   |
| 1   | B     | 312  | GLU  | N-CA-C    | -7.49 | 102.05      | 112.45   |
| 1   | A     | 1004 | VAL  | N-CA-C    | 7.42  | 118.97      | 108.36   |
| 1   | B     | 186  | GLN  | CG-CD-NE2 | 7.41  | 127.52      | 116.40   |
| 1   | B     | 455  | GLN  | CG-CD-NE2 | 7.40  | 127.50      | 116.40   |
| 1   | A     | 562  | THR  | N-CA-C    | 7.39  | 120.77      | 111.24   |
| 1   | B     | 598  | SER  | N-CA-C    | -7.37 | 101.13      | 112.99   |
| 2   | D     | 112  | GLN  | CG-CD-NE2 | 7.30  | 127.35      | 116.40   |
| 2   | C     | 190  | CYS  | O-C-N     | 7.29  | 132.47      | 123.21   |
| 1   | A     | 930  | VAL  | N-CA-C    | 7.28  | 117.99      | 110.05   |
| 1   | A     | 35   | LYS  | CB-CA-C   | 7.25  | 124.85      | 110.42   |
| 2   | D     | 211  | CYS  | CA-C-N    | 7.22  | 128.87      | 119.84   |
| 2   | D     | 211  | CYS  | C-N-CA    | 7.22  | 128.87      | 119.84   |
| 1   | B     | 36   | ASN  | N-CA-C    | -7.19 | 95.49       | 110.80   |
| 1   | B     | 746  | SER  | CB-CA-C   | -7.19 | 100.31      | 111.74   |
| 1   | B     | 378  | CYS  | N-CA-C    | -7.19 | 97.02       | 108.73   |
| 1   | B     | 467  | GLN  | CG-CD-NE2 | 7.18  | 127.17      | 116.40   |
| 2   | C     | 53   | ASN  | CB-CA-C   | 7.17  | 122.35      | 110.88   |
| 1   | A     | 290  | GLN  | CG-CD-NE2 | 7.07  | 127.00      | 116.40   |
| 1   | B     | 895  | THR  | N-CA-C    | -7.05 | 103.61      | 111.71   |
| 1   | A     | 370  | GLN  | CG-CD-NE2 | 6.99  | 126.89      | 116.40   |
| 1   | A     | 597  | GLU  | N-CA-C    | -6.98 | 100.94      | 111.34   |
| 1   | A     | 211  | ASN  | N-CA-C    | 6.97  | 119.06      | 110.91   |
| 1   | B     | 449  | MET  | O-C-N     | 6.96  | 129.27      | 122.03   |
| 1   | B     | 222  | VAL  | CA-C-N    | 6.90  | 128.47      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 222  | VAL  | C-N-CA    | 6.90  | 128.47      | 119.84   |
| 1   | A     | 902  | GLU  | CA-CB-CG  | 6.87  | 127.83      | 114.10   |
| 1   | B     | 82   | ALA  | N-CA-C    | -6.85 | 104.19      | 112.54   |
| 1   | B     | 743  | GLN  | CG-CD-NE2 | 6.81  | 126.62      | 116.40   |
| 2   | C     | 212  | PRO  | N-CA-C    | 6.81  | 121.07      | 111.33   |
| 1   | B     | 108  | VAL  | N-CA-C    | 6.78  | 118.82      | 111.77   |
| 1   | A     | 698  | THR  | N-CA-C    | 6.76  | 120.18      | 109.50   |
| 1   | A     | 861  | VAL  | N-CA-C    | 6.76  | 116.85      | 110.30   |
| 1   | B     | 463  | VAL  | CA-C-N    | 6.74  | 134.41      | 121.54   |
| 1   | B     | 463  | VAL  | C-N-CA    | 6.74  | 134.41      | 121.54   |
| 2   | D     | 17   | ILE  | N-CA-C    | -6.74 | 96.57       | 107.28   |
| 1   | A     | 96   | GLU  | N-CA-C    | -6.72 | 105.19      | 113.19   |
| 1   | B     | 456  | GLN  | CG-CD-NE2 | 6.72  | 126.48      | 116.40   |
| 1   | A     | 117  | GLU  | N-CA-C    | -6.69 | 99.36       | 109.60   |
| 1   | B     | 432  | GLN  | CG-CD-NE2 | 6.67  | 126.41      | 116.40   |
| 1   | B     | 332  | GLN  | N-CA-C    | 6.66  | 118.88      | 108.96   |
| 1   | B     | 466  | GLN  | CG-CD-NE2 | 6.63  | 126.35      | 116.40   |
| 1   | A     | 902  | GLU  | N-CA-C    | -6.58 | 96.79       | 110.80   |
| 2   | D     | 102  | LEU  | N-CA-CB   | -6.53 | 99.46       | 110.49   |
| 1   | A     | 36   | ASN  | CA-CB-CG  | 6.50  | 119.10      | 112.60   |
| 2   | D     | 195  | SER  | CA-C-N    | 6.50  | 126.41      | 119.85   |
| 2   | D     | 195  | SER  | C-N-CA    | 6.50  | 126.41      | 119.85   |
| 1   | B     | 416  | ASP  | CA-C-N    | 6.49  | 126.18      | 119.56   |
| 1   | B     | 416  | ASP  | C-N-CA    | 6.49  | 126.18      | 119.56   |
| 1   | A     | 687  | TYR  | CA-C-N    | 6.46  | 126.81      | 119.83   |
| 1   | A     | 687  | TYR  | C-N-CA    | 6.46  | 126.81      | 119.83   |
| 1   | A     | 708  | GLN  | CG-CD-NE2 | 6.46  | 126.08      | 116.40   |
| 1   | A     | 595  | THR  | CA-C-N    | -6.44 | 110.49      | 122.60   |
| 1   | A     | 595  | THR  | C-N-CA    | -6.44 | 110.49      | 122.60   |
| 1   | B     | 1006 | VAL  | N-CA-C    | 6.43  | 116.29      | 108.06   |
| 1   | B     | 370  | GLN  | CG-CD-NE2 | 6.41  | 126.02      | 116.40   |
| 1   | A     | 573  | SER  | N-CA-C    | 6.40  | 121.09      | 113.16   |
| 2   | C     | 37   | SER  | N-CA-CB   | 6.36  | 120.66      | 110.86   |
| 2   | D     | 182  | ASP  | CA-CB-CG  | -6.35 | 106.25      | 112.60   |
| 1   | B     | 327  | ARG  | N-CA-C    | -6.35 | 106.12      | 114.31   |
| 2   | C     | 216  | SER  | N-CA-C    | -6.33 | 104.82      | 113.30   |
| 1   | A     | 706  | GLU  | CA-C-N    | -6.30 | 113.52      | 121.96   |
| 1   | A     | 706  | GLU  | C-N-CA    | -6.30 | 113.52      | 121.96   |
| 1   | B     | 615  | GLY  | N-CA-C    | -6.29 | 101.77      | 111.64   |
| 1   | B     | 118  | THR  | N-CA-C    | -6.28 | 106.15      | 113.88   |
| 1   | A     | 382  | PHE  | CB-CA-C   | -6.27 | 109.33      | 116.54   |
| 1   | B     | 455  | GLN  | CB-CA-C   | 6.23  | 122.82      | 110.42   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 205  | GLY  | CA-C-N   | 6.22  | 127.62      | 119.84   |
| 1   | A     | 205  | GLY  | C-N-CA   | 6.22  | 127.62      | 119.84   |
| 1   | B     | 429  | PHE  | CB-CA-C  | -6.20 | 101.50      | 111.86   |
| 2   | C     | 206  | CYS  | N-CA-C   | 6.19  | 119.56      | 109.59   |
| 1   | A     | 290  | GLN  | CB-CG-CD | 6.18  | 123.11      | 112.60   |
| 1   | B     | 449  | MET  | CA-C-N   | 6.14  | 133.45      | 121.41   |
| 1   | B     | 449  | MET  | C-N-CA   | 6.14  | 133.45      | 121.41   |
| 1   | B     | 747  | GLY  | O-C-N    | 6.13  | 130.67      | 122.70   |
| 2   | C     | 53   | ASN  | CA-C-O   | 6.07  | 128.00      | 121.02   |
| 1   | B     | 743  | GLN  | CA-C-N   | 6.04  | 131.41      | 121.39   |
| 1   | B     | 743  | GLN  | C-N-CA   | 6.04  | 131.41      | 121.39   |
| 2   | D     | 118  | SER  | N-CA-C   | -6.01 | 105.90      | 113.18   |
| 1   | A     | 902  | GLU  | N-CA-CB  | 5.99  | 120.61      | 110.49   |
| 1   | B     | 1126 | ALA  | N-CA-C   | -5.98 | 104.88      | 111.82   |
| 1   | A     | 1006 | VAL  | N-CA-C   | 5.97  | 117.28      | 108.45   |
| 1   | A     | 413  | LEU  | N-CA-C   | 5.93  | 118.30      | 108.99   |
| 1   | B     | 464  | ALA  | N-CA-C   | 5.93  | 123.43      | 110.80   |
| 1   | B     | 837  | TYR  | CA-C-N   | 5.93  | 127.25      | 119.84   |
| 1   | B     | 837  | TYR  | C-N-CA   | 5.93  | 127.25      | 119.84   |
| 1   | A     | 902  | GLU  | CB-CG-CD | -5.91 | 102.55      | 112.60   |
| 1   | A     | 347  | VAL  | N-CA-C   | 5.88  | 117.22      | 108.23   |
| 1   | A     | 895  | THR  | N-CA-C   | -5.87 | 106.07      | 113.18   |
| 1   | B     | 429  | PHE  | CA-C-N   | -5.86 | 111.42      | 121.97   |
| 1   | B     | 429  | PHE  | C-N-CA   | -5.86 | 111.42      | 121.97   |
| 2   | C     | 139  | ASN  | CA-C-N   | -5.83 | 113.25      | 122.23   |
| 2   | C     | 139  | ASN  | C-N-CA   | -5.83 | 113.25      | 122.23   |
| 2   | C     | 177  | ILE  | N-CA-C   | 5.83  | 117.14      | 108.46   |
| 1   | B     | 942  | PHE  | N-CA-C   | 5.81  | 119.85      | 107.70   |
| 1   | A     | 501  | ALA  | N-CA-C   | 5.78  | 117.80      | 107.80   |
| 1   | B     | 645  | SER  | N-CA-C   | -5.78 | 107.47      | 114.75   |
| 1   | B     | 420  | GLU  | N-CA-C   | -5.77 | 104.59      | 111.69   |
| 1   | A     | 309  | SER  | N-CA-C   | -5.76 | 102.77      | 110.55   |
| 1   | A     | 34   | ALA  | CA-C-N   | -5.75 | 110.55      | 121.54   |
| 1   | A     | 34   | ALA  | C-N-CA   | -5.75 | 110.55      | 121.54   |
| 1   | A     | 1092 | ASP  | N-CA-C   | -5.74 | 104.94      | 111.14   |
| 2   | C     | 53   | ASN  | O-C-N    | 5.72  | 130.26      | 122.48   |
| 2   | C     | 194  | CYS  | CA-CB-SG | 5.71  | 127.52      | 114.40   |
| 1   | A     | 370  | GLN  | CB-CG-CD | 5.67  | 122.25      | 112.60   |
| 1   | B     | 413  | LEU  | N-CA-C   | 5.67  | 117.13      | 108.52   |
| 1   | B     | 901  | THR  | N-CA-C   | 5.67  | 118.23      | 110.24   |
| 1   | B     | 831  | VAL  | N-CA-C   | 5.66  | 116.04      | 108.11   |
| 1   | A     | 836  | VAL  | N-CA-C   | 5.66  | 116.25      | 107.99   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 465  | HIS  | CB-CA-C  | -5.65 | 99.17       | 110.42   |
| 2   | C     | 138  | GLU  | N-CA-C   | 5.65  | 117.44      | 111.28   |
| 1   | A     | 862  | ALA  | N-CA-C   | 5.64  | 116.81      | 108.86   |
| 1   | A     | 615  | GLY  | N-CA-C   | -5.63 | 102.81      | 111.64   |
| 1   | B     | 555  | LEU  | N-CA-C   | 5.61  | 118.61      | 109.24   |
| 2   | C     | 53   | ASN  | CA-CB-CG | -5.60 | 107.00      | 112.60   |
| 1   | B     | 1053 | ASP  | N-CA-C   | -5.57 | 105.12      | 111.14   |
| 1   | B     | 1045 | GLU  | N-CA-C   | -5.57 | 105.75      | 112.54   |
| 1   | A     | 530  | SER  | N-CA-C   | 5.56  | 115.18      | 107.73   |
| 2   | D     | 124  | SER  | N-CA-C   | 5.54  | 116.82      | 108.46   |
| 1   | A     | 837  | TYR  | CA-C-N   | 5.50  | 125.85      | 119.47   |
| 1   | A     | 837  | TYR  | C-N-CA   | 5.50  | 125.85      | 119.47   |
| 1   | A     | 435  | VAL  | N-CA-C   | 5.47  | 115.66      | 107.51   |
| 1   | A     | 49   | LEU  | N-CA-C   | 5.46  | 117.62      | 108.73   |
| 2   | D     | 208  | CYS  | CA-CB-SG | 5.45  | 126.93      | 114.40   |
| 1   | B     | 195  | VAL  | N-CA-C   | 5.44  | 115.96      | 108.12   |
| 1   | B     | 84   | TYR  | N-CA-C   | 5.44  | 119.21      | 112.58   |
| 1   | B     | 455  | GLN  | CA-CB-CG | -5.42 | 103.26      | 114.10   |
| 1   | B     | 720  | SER  | N-CA-C   | 5.41  | 119.24      | 109.44   |
| 1   | A     | 119  | GLY  | N-CA-C   | 5.41  | 125.99      | 113.18   |
| 1   | B     | 587  | ILE  | CA-C-N   | 5.41  | 126.25      | 119.98   |
| 1   | B     | 587  | ILE  | C-N-CA   | 5.41  | 126.25      | 119.98   |
| 1   | A     | 120  | ILE  | N-CA-C   | 5.38  | 115.94      | 108.84   |
| 2   | D     | 177  | ILE  | N-CA-C   | 5.38  | 117.13      | 108.85   |
| 2   | C     | 172  | ARG  | CA-C-N   | 5.36  | 128.96      | 121.24   |
| 2   | C     | 172  | ARG  | C-N-CA   | 5.36  | 128.96      | 121.24   |
| 1   | B     | 1092 | ASP  | N-CA-C   | -5.36 | 105.36      | 111.14   |
| 2   | C     | 108  | THR  | CA-C-N   | -5.33 | 113.18      | 119.84   |
| 2   | C     | 108  | THR  | C-N-CA   | -5.33 | 113.18      | 119.84   |
| 1   | B     | 465  | HIS  | N-CA-CB  | 5.31  | 119.46      | 110.49   |
| 1   | A     | 418  | ASN  | N-CA-C   | 5.29  | 118.07      | 111.24   |
| 1   | B     | 970  | ASN  | N-CA-C   | 5.29  | 119.48      | 113.19   |
| 1   | A     | 699  | LEU  | N-CA-C   | -5.28 | 102.70      | 110.52   |
| 1   | A     | 1072 | PHE  | N-CA-C   | -5.27 | 105.44      | 111.14   |
| 1   | B     | 308  | THR  | CB-CA-C  | -5.25 | 109.50      | 117.07   |
| 1   | A     | 223  | PRO  | N-CA-C   | 5.24  | 118.82      | 111.33   |
| 1   | A     | 332  | GLN  | N-CA-C   | 5.22  | 116.74      | 108.96   |
| 1   | A     | 833  | THR  | N-CA-C   | 5.22  | 116.22      | 108.86   |
| 1   | B     | 1004 | VAL  | N-CA-C   | 5.21  | 115.82      | 109.30   |
| 1   | A     | 887  | THR  | N-CA-C   | 5.21  | 118.05      | 109.72   |
| 1   | B     | 913  | TYR  | N-CA-C   | 5.20  | 117.37      | 108.90   |
| 1   | B     | 912  | LEU  | N-CA-C   | 5.19  | 118.77      | 112.23   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 749  | THR  | CB-CA-C   | 5.18  | 119.18      | 109.86   |
| 1   | B     | 366  | ASP  | CA-C-N    | 5.17  | 129.48      | 121.26   |
| 1   | B     | 366  | ASP  | C-N-CA    | 5.17  | 129.48      | 121.26   |
| 1   | A     | 1076 | PHE  | N-CA-C    | -5.16 | 102.96      | 110.24   |
| 2   | D     | 147  | GLU  | CA-C-N    | 5.16  | 126.29      | 119.84   |
| 2   | D     | 147  | GLU  | C-N-CA    | 5.16  | 126.29      | 119.84   |
| 1   | A     | 1065 | VAL  | N-CA-C    | 5.15  | 120.05      | 109.34   |
| 1   | A     | 844  | LYS  | N-CA-C    | -5.14 | 106.97      | 114.12   |
| 1   | A     | 566  | ALA  | N-CA-C    | -5.13 | 100.54      | 108.90   |
| 1   | A     | 7    | VAL  | CB-CA-C   | -5.12 | 102.49      | 110.69   |
| 1   | A     | 207  | TRP  | N-CA-C    | 5.12  | 117.20      | 109.41   |
| 1   | A     | 222  | VAL  | CA-C-N    | 5.12  | 125.84      | 120.11   |
| 1   | A     | 222  | VAL  | C-N-CA    | 5.12  | 125.84      | 120.11   |
| 1   | A     | 903  | CYS  | N-CA-C    | 5.11  | 118.00      | 110.59   |
| 1   | B     | 404  | LEU  | CA-C-N    | 5.10  | 125.00      | 119.85   |
| 1   | B     | 404  | LEU  | C-N-CA    | 5.10  | 125.00      | 119.85   |
| 1   | B     | 780  | THR  | CA-C-N    | 5.09  | 131.26      | 121.54   |
| 1   | B     | 780  | THR  | C-N-CA    | 5.09  | 131.26      | 121.54   |
| 1   | B     | 989  | ARG  | N-CA-C    | -5.09 | 107.03      | 113.18   |
| 1   | A     | 541  | LEU  | N-CA-C    | 5.08  | 117.11      | 109.23   |
| 1   | B     | 1105 | MET  | N-CA-C    | -5.07 | 105.94      | 111.82   |
| 1   | A     | 377  | THR  | N-CA-C    | 5.07  | 117.85      | 109.85   |
| 1   | B     | 451  | PHE  | CB-CG-CD1 | -5.05 | 112.11      | 120.70   |
| 1   | A     | 87   | CYS  | N-CA-C    | 5.04  | 116.19      | 108.42   |
| 1   | B     | 162  | LEU  | N-CA-C    | 5.04  | 116.62      | 111.03   |
| 1   | A     | 505  | SER  | N-CA-C    | 5.04  | 117.50      | 111.71   |
| 2   | D     | 100  | ASN  | N-CA-C    | -5.03 | 103.74      | 110.07   |
| 1   | B     | 744  | ASP  | CA-C-N    | -5.00 | 112.38      | 121.14   |
| 1   | B     | 744  | ASP  | C-N-CA    | -5.00 | 112.38      | 121.14   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | B     | 1   | MET  | CA   |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 430 | VAL  | Peptide   |
| 2   | D     | 190 | CYS  | Mainchain |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 8860  | 0        | 8828     | 495     | 0            |
| 1   | B     | 8876  | 0        | 8842     | 826     | 0            |
| 2   | C     | 1324  | 0        | 1306     | 134     | 0            |
| 2   | D     | 1335  | 0        | 1323     | 179     | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 20399 | 0        | 20299    | 1618    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (1618) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CG   | 1.51                     | 1.38              |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CB   | 1.50                     | 1.37              |
| 1:B:367:LEU:CD2  | 1:B:374:GLN:HB2  | 1.53                     | 1.37              |
| 1:B:742:VAL:CG2  | 1:B:750:THR:HG21 | 1.57                     | 1.35              |
| 1:B:367:LEU:CD2  | 1:B:374:GLN:CG   | 2.06                     | 1.34              |
| 1:B:367:LEU:HD13 | 1:B:374:GLN:CD   | 1.51                     | 1.33              |
| 2:D:169:GLY:O    | 2:D:212:PRO:CD   | 1.75                     | 1.33              |
| 1:B:367:LEU:CD2  | 1:B:374:GLN:CB   | 2.08                     | 1.31              |
| 1:B:367:LEU:CD1  | 1:B:374:GLN:OE1  | 1.79                     | 1.31              |
| 1:B:432:GLN:OE1  | 1:B:454:ASP:CB   | 1.79                     | 1.31              |
| 1:B:367:LEU:O    | 1:B:368:GLU:HG2  | 1.12                     | 1.29              |
| 2:D:169:GLY:O    | 2:D:212:PRO:HD2  | 1.28                     | 1.27              |
| 2:D:190:CYS:SG   | 2:D:218:CYS:HB3  | 1.80                     | 1.22              |
| 1:B:369:ARG:HB2  | 1:B:655:ARG:HH12 | 1.07                     | 1.19              |
| 1:A:289:GLU:O    | 1:A:290:GLN:O    | 1.55                     | 1.19              |
| 1:A:660:TYR:OH   | 1:A:708:GLN:OE1  | 1.58                     | 1.19              |
| 1:B:750:THR:O    | 1:B:750:THR:CG2  | 1.79                     | 1.19              |
| 2:D:170:PHE:O    | 2:D:193:SER:HB3  | 1.40                     | 1.19              |
| 1:A:16:ASN:ND2   | 1:A:35:LYS:O     | 1.74                     | 1.19              |
| 2:C:35:THR:HG22  | 2:C:36:SER:O     | 1.38                     | 1.18              |
| 1:B:742:VAL:CG2  | 1:B:750:THR:CG2  | 2.21                     | 1.18              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:367:LEU:HD13 | 1:B:374:GLN:OE1   | 1.02                     | 1.18              |
| 1:B:367:LEU:CD1  | 1:B:374:GLN:CD    | 2.12                     | 1.18              |
| 1:B:367:LEU:CD2  | 1:B:374:GLN:HG3   | 1.72                     | 1.17              |
| 1:B:367:LEU:O    | 1:B:368:GLU:CG    | 1.90                     | 1.17              |
| 1:B:474:ALA:HB3  | 1:B:477:ARG:HH22  | 1.08                     | 1.14              |
| 1:B:432:GLN:OE1  | 1:B:454:ASP:HB3   | 0.97                     | 1.12              |
| 1:B:889:ARG:HD3  | 1:B:904:ASN:HD21  | 0.98                     | 1.10              |
| 1:B:742:VAL:HG23 | 1:B:750:THR:HG21  | 1.18                     | 1.08              |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:HG3   | 1.18                     | 1.08              |
| 1:B:456:GLN:NE2  | 1:B:473:SER:OG    | 1.86                     | 1.07              |
| 1:A:81:THR:HG22  | 1:A:83:LYS:H      | 1.19                     | 1.07              |
| 1:B:286:GLU:HB2  | 1:B:299:ASP:H     | 1.17                     | 1.07              |
| 2:C:52:THR:O     | 2:C:52:THR:HG22   | 1.52                     | 1.07              |
| 1:B:368:GLU:OE1  | 1:B:391:ARG:NH2   | 1.88                     | 1.06              |
| 1:B:367:LEU:HD11 | 1:B:374:GLN:HG3   | 1.37                     | 1.06              |
| 2:D:111:THR:O    | 2:D:188:GLU:OE2   | 1.74                     | 1.05              |
| 1:B:456:GLN:NE2  | 1:B:473:SER:CB    | 2.20                     | 1.05              |
| 1:B:742:VAL:HG23 | 1:B:750:THR:CG2   | 1.83                     | 1.05              |
| 1:A:371:GLY:HA3  | 1:A:1016:ASN:HD21 | 1.13                     | 1.05              |
| 1:A:889:ARG:HD3  | 1:A:904:ASN:HD21  | 1.16                     | 1.04              |
| 1:B:367:LEU:CD1  | 1:B:374:GLN:HG3   | 1.86                     | 1.04              |
| 1:B:367:LEU:CD1  | 1:B:374:GLN:CG    | 2.35                     | 1.03              |
| 1:B:81:THR:HG22  | 1:B:83:LYS:H      | 1.22                     | 1.03              |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:HB2   | 1.40                     | 1.03              |
| 1:B:367:LEU:HD11 | 1:B:374:GLN:CG    | 1.89                     | 1.03              |
| 1:A:167:VAL:HG13 | 1:A:180:PHE:HB3   | 1.38                     | 1.02              |
| 1:B:449:MET:HE2  | 1:B:449:MET:HA    | 1.42                     | 1.01              |
| 1:B:450:GLY:HA3  | 1:B:479:VAL:HG11  | 1.42                     | 1.01              |
| 1:B:367:LEU:HD12 | 1:B:368:GLU:HG2   | 1.44                     | 1.00              |
| 1:B:368:GLU:CD   | 1:B:391:ARG:NH2   | 2.20                     | 0.99              |
| 1:B:267:ASN:HD21 | 1:B:269:SER:HB2   | 1.26                     | 0.98              |
| 1:A:23:PHE:H     | 1:A:30:ASN:HD22   | 1.00                     | 0.98              |
| 1:B:482:GLU:HB2  | 1:B:483:PRO:HD3   | 1.43                     | 0.98              |
| 2:C:112:GLN:HE22 | 2:C:187:THR:HG23  | 1.28                     | 0.98              |
| 1:B:1105:MET:HE3 | 1:B:1126:ALA:HB1  | 1.43                     | 0.98              |
| 2:D:143:ARG:HB3  | 2:D:143:ARG:CZ    | 1.89                     | 0.98              |
| 2:C:52:THR:HG21  | 2:C:85:ILE:HG12   | 1.43                     | 0.97              |
| 1:B:178:ILE:HG22 | 1:B:193:TYR:O     | 1.65                     | 0.97              |
| 1:B:167:VAL:HG12 | 1:B:180:PHE:HB3   | 1.47                     | 0.97              |
| 1:B:288:GLU:HB2  | 1:B:298:LYS:HB2   | 1.45                     | 0.97              |
| 1:A:706:GLU:O    | 1:A:707:ILE:HG13  | 1.63                     | 0.96              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:504:ASN:HD21  | 1:A:507:GLN:HE21 | 1.02                     | 0.96              |
| 1:B:23:PHE:H      | 1:B:30:ASN:HD22  | 1.03                     | 0.96              |
| 1:B:889:ARG:HD3   | 1:B:904:ASN:ND2  | 1.81                     | 0.96              |
| 1:B:191:LYS:HG2   | 1:B:192:THR:H    | 1.30                     | 0.96              |
| 1:A:356:LEU:HD21  | 1:A:712:ILE:HD13 | 1.48                     | 0.95              |
| 1:B:367:LEU:CG    | 1:B:374:GLN:HG3  | 1.97                     | 0.95              |
| 1:B:294:THR:HG22  | 1:B:295:VAL:H    | 1.30                     | 0.94              |
| 1:B:24:THR:H      | 1:B:30:ASN:HD21  | 1.12                     | 0.94              |
| 1:B:368:GLU:OE2   | 1:B:391:ARG:NH2  | 2.01                     | 0.93              |
| 1:A:889:ARG:HD3   | 1:A:904:ASN:ND2  | 1.83                     | 0.93              |
| 2:D:171:HIS:NE2   | 2:D:212:PRO:HG2  | 1.84                     | 0.93              |
| 1:B:478:LEU:HD23  | 1:B:479:VAL:H    | 1.31                     | 0.92              |
| 2:C:190:CYS:HB2   | 2:C:218:CYS:SG   | 2.09                     | 0.92              |
| 2:C:208:CYS:SG    | 2:C:210:GLN:HG2  | 2.09                     | 0.92              |
| 1:B:456:GLN:CD    | 1:B:473:SER:HB3  | 1.94                     | 0.92              |
| 1:B:976:VAL:HG22  | 1:B:996:GLY:HA3  | 1.50                     | 0.92              |
| 1:B:286:GLU:HG3   | 1:B:299:ASP:HB3  | 1.52                     | 0.91              |
| 1:B:474:ALA:HB3   | 1:B:477:ARG:NH2  | 1.85                     | 0.91              |
| 1:B:480:SER:HB3   | 1:B:485:ALA:H    | 1.36                     | 0.91              |
| 2:C:194:CYS:SG    | 2:C:208:CYS:N    | 2.42                     | 0.91              |
| 1:B:450:GLY:O     | 1:B:479:VAL:HG21 | 1.70                     | 0.91              |
| 2:D:108:THR:O     | 2:D:110:SER:N    | 2.04                     | 0.91              |
| 2:D:80:ARG:HB2    | 2:D:81:PRO:HD3   | 1.51                     | 0.90              |
| 1:A:660:TYR:HH    | 1:A:708:GLN:CD   | 1.79                     | 0.90              |
| 2:C:52:THR:CG2    | 2:C:85:ILE:HG23  | 2.01                     | 0.90              |
| 1:B:162:LEU:HD23  | 1:B:162:LEU:H    | 1.35                     | 0.90              |
| 1:B:1125:THR:HG22 | 1:B:1127:ASP:H   | 1.34                     | 0.90              |
| 1:B:742:VAL:O     | 1:B:750:THR:HB   | 1.71                     | 0.90              |
| 1:B:478:LEU:HD23  | 1:B:479:VAL:N    | 1.87                     | 0.90              |
| 1:B:225:PRO:HG2   | 1:B:267:ASN:HB2  | 1.53                     | 0.89              |
| 1:B:450:GLY:HA3   | 1:B:479:VAL:CG1  | 2.01                     | 0.89              |
| 1:A:422:TYR:HD1   | 1:A:683:ASN:H    | 1.11                     | 0.89              |
| 1:B:1032:THR:HG22 | 1:B:1034:ASN:H   | 1.35                     | 0.89              |
| 1:B:256:SER:HB2   | 1:B:276:MET:HB3  | 1.53                     | 0.89              |
| 2:C:109:PRO:HG2   | 2:C:203:ARG:CZ   | 2.02                     | 0.89              |
| 2:D:190:CYS:SG    | 2:D:218:CYS:CB   | 2.47                     | 0.89              |
| 1:A:889:ARG:HH11  | 1:A:904:ASN:ND2  | 1.69                     | 0.88              |
| 1:B:432:GLN:CD    | 1:B:454:ASP:HB3  | 1.98                     | 0.88              |
| 1:B:594:THR:HG22  | 1:B:595:THR:H    | 1.36                     | 0.88              |
| 2:C:52:THR:HG21   | 2:C:85:ILE:HG23  | 1.54                     | 0.88              |
| 1:B:453:ASP:OD2   | 1:B:472:THR:HG21 | 1.73                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:24:THR:H     | 1:B:30:ASN:ND2   | 1.70                     | 0.88              |
| 1:A:253:ILE:HD12 | 1:A:258:ILE:HD11 | 1.55                     | 0.87              |
| 2:D:169:GLY:O    | 2:D:212:PRO:HD3  | 1.71                     | 0.87              |
| 1:B:451:PHE:C    | 1:B:451:PHE:CD2  | 2.52                     | 0.87              |
| 1:B:570:LYS:HG3  | 1:B:572:PRO:HD2  | 1.56                     | 0.87              |
| 2:C:52:THR:O     | 2:C:54:ALA:N     | 2.07                     | 0.87              |
| 1:B:178:ILE:CG2  | 1:B:193:TYR:O    | 2.22                     | 0.87              |
| 1:B:232:ILE:HG21 | 1:B:258:ILE:HD12 | 1.56                     | 0.87              |
| 1:B:746:SER:OG   | 1:B:746:SER:O    | 1.78                     | 0.87              |
| 2:C:52:THR:HG21  | 2:C:85:ILE:CG1   | 2.05                     | 0.87              |
| 1:A:699:LEU:HD13 | 1:A:700:THR:N    | 1.90                     | 0.86              |
| 1:A:396:ILE:HD13 | 1:A:396:ILE:H    | 1.38                     | 0.86              |
| 1:B:507:GLN:HE22 | 1:B:553:SER:H    | 1.22                     | 0.86              |
| 1:B:430:VAL:HG13 | 1:B:456:GLN:HB3  | 1.55                     | 0.86              |
| 1:B:367:LEU:C    | 1:B:368:GLU:HG2  | 2.01                     | 0.86              |
| 1:B:790:ASN:HB3  | 1:B:806:GLN:HA   | 1.59                     | 0.85              |
| 1:B:404:LEU:O    | 1:B:407:ILE:HD11 | 1.75                     | 0.85              |
| 2:C:194:CYS:SG   | 2:C:207:THR:N    | 2.49                     | 0.85              |
| 2:D:171:HIS:HB2  | 2:D:215:CYS:CB   | 2.06                     | 0.85              |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CG   | 2.07                     | 0.85              |
| 1:B:436:LEU:HD12 | 1:B:445:GLU:HB3  | 1.59                     | 0.85              |
| 1:B:869:ALA:O    | 1:B:884:ILE:O    | 1.94                     | 0.85              |
| 1:B:433:THR:HG21 | 1:B:457:THR:OG1  | 1.76                     | 0.85              |
| 1:B:329:GLY:HA3  | 1:B:384:GLU:HG2  | 1.59                     | 0.84              |
| 1:B:369:ARG:HB2  | 1:B:655:ARG:NH1  | 1.92                     | 0.84              |
| 1:B:994:GLU:O    | 1:B:995:VAL:HG22 | 1.78                     | 0.84              |
| 1:A:743:GLN:HA   | 1:A:749:THR:HG22 | 1.59                     | 0.84              |
| 1:A:23:PHE:H     | 1:A:30:ASN:ND2   | 1.74                     | 0.83              |
| 1:A:553:SER:O    | 1:A:571:LEU:HD12 | 1.79                     | 0.83              |
| 1:B:742:VAL:HG21 | 1:B:750:THR:HG21 | 1.60                     | 0.83              |
| 2:C:51:LEU:HD22  | 2:C:142:THR:H    | 1.43                     | 0.83              |
| 1:B:742:VAL:HG22 | 1:B:750:THR:CG2  | 2.09                     | 0.83              |
| 1:A:24:THR:H     | 1:A:30:ASN:HD21  | 1.25                     | 0.83              |
| 1:A:417:PRO:HG3  | 1:A:481:GLN:HB3  | 1.61                     | 0.82              |
| 1:B:731:GLN:HA   | 1:B:796:GLN:NE2  | 1.94                     | 0.82              |
| 1:B:756:ALA:HB1  | 1:B:801:VAL:HG21 | 1.61                     | 0.82              |
| 1:A:186:GLN:H    | 1:A:186:GLN:HE21 | 1.28                     | 0.82              |
| 1:B:255:GLN:H    | 1:B:255:GLN:HE21 | 1.28                     | 0.82              |
| 1:B:10:GLN:HB3   | 1:B:1037:ILE:HB  | 1.61                     | 0.82              |
| 2:C:168:GLY:HA2  | 2:C:193:SER:HB2  | 1.61                     | 0.82              |
| 1:A:780:THR:O    | 1:A:781:SER:O    | 1.96                     | 0.81              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1032:THR:HG23 | 1:A:1034:ASN:H   | 1.44                     | 0.81              |
| 1:B:981:SER:HA    | 1:B:989:ARG:HG3  | 1.63                     | 0.81              |
| 1:B:367:LEU:O     | 1:B:367:LEU:HD12 | 1.80                     | 0.81              |
| 1:B:437:MET:HB3   | 1:B:444:GLU:O    | 1.80                     | 0.81              |
| 2:D:114:VAL:HG22  | 2:D:185:LYS:HD3  | 1.62                     | 0.81              |
| 1:B:803:HIS:HD2   | 1:B:804:ALA:H    | 1.29                     | 0.81              |
| 2:C:190:CYS:CB    | 2:C:218:CYS:SG   | 2.69                     | 0.81              |
| 1:B:290:GLN:HE21  | 1:B:293:GLY:HA3  | 1.43                     | 0.80              |
| 2:D:88:ALA:HA     | 2:D:199:ALA:HB3  | 1.61                     | 0.80              |
| 1:A:81:THR:HG22   | 1:A:83:LYS:N     | 1.96                     | 0.80              |
| 1:B:25:SER:O      | 1:B:74:LYS:HB3   | 1.82                     | 0.80              |
| 1:B:297:LEU:HD21  | 1:B:300:LEU:HD11 | 1.63                     | 0.80              |
| 1:A:705:ASP:OD2   | 1:A:709:LYS:HE2  | 1.82                     | 0.80              |
| 1:B:476:VAL:HG13  | 1:B:490:TRP:HB3  | 1.64                     | 0.80              |
| 2:C:112:GLN:NE2   | 2:C:187:THR:HG23 | 1.96                     | 0.80              |
| 1:B:1101:SER:OG   | 1:B:1103:PRO:HD2 | 1.80                     | 0.80              |
| 2:D:192:PRO:O     | 2:D:194:CYS:N    | 2.15                     | 0.80              |
| 1:B:275:ASP:HB2   | 1:B:279:ARG:H    | 1.45                     | 0.79              |
| 1:B:466:GLN:O     | 1:B:481:GLN:HB2  | 1.82                     | 0.79              |
| 1:A:146:ASP:C     | 1:A:148:ASP:H    | 1.89                     | 0.79              |
| 1:B:139:LEU:HB3   | 1:B:156:ASN:HD22 | 1.45                     | 0.79              |
| 1:B:750:THR:O     | 1:B:750:THR:HG22 | 1.01                     | 0.79              |
| 2:D:116:ASP:O     | 2:D:182:ASP:HB3  | 1.83                     | 0.78              |
| 1:A:454:ASP:O     | 1:A:455:GLN:HG2  | 1.83                     | 0.78              |
| 1:A:889:ARG:HH11  | 1:A:904:ASN:HD21 | 1.27                     | 0.78              |
| 1:A:416:ASP:HB3   | 1:A:419:ARG:HG3  | 1.66                     | 0.78              |
| 1:B:894:THR:HG22  | 1:B:896:GLU:H    | 1.49                     | 0.78              |
| 1:A:112:ILE:HD13  | 1:A:112:ILE:H    | 1.46                     | 0.78              |
| 1:B:419:ARG:HH11  | 1:B:423:ASP:HB3  | 1.48                     | 0.78              |
| 1:B:47:GLU:HG2    | 1:B:48:GLY:H     | 1.48                     | 0.78              |
| 1:A:186:GLN:H     | 1:A:186:GLN:NE2  | 1.81                     | 0.78              |
| 1:A:24:THR:H      | 1:A:30:ASN:ND2   | 1.81                     | 0.77              |
| 1:B:432:GLN:OE1   | 1:B:454:ASP:CA   | 2.32                     | 0.77              |
| 1:A:429:PHE:O     | 1:A:456:GLN:HG3  | 1.84                     | 0.77              |
| 1:A:706:GLU:O     | 1:A:707:ILE:CG1  | 2.31                     | 0.77              |
| 1:B:57:MET:HE3    | 1:B:1066:GLY:H   | 1.49                     | 0.77              |
| 1:B:367:LEU:CD2   | 1:B:374:GLN:CD   | 2.56                     | 0.77              |
| 1:A:143:ILE:HG12  | 1:A:154:ALA:HB2  | 1.66                     | 0.77              |
| 1:A:440:GLY:O     | 1:A:686:GLY:HA3  | 1.82                     | 0.77              |
| 2:C:52:THR:O      | 2:C:52:THR:CG2   | 2.24                     | 0.77              |
| 2:C:52:THR:HG21   | 2:C:85:ILE:CG2   | 2.15                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:ARG:HD3   | 1:A:75:ASP:OD2   | 1.84                     | 0.77              |
| 1:A:504:ASN:HD21 | 1:A:507:GLN:NE2  | 1.81                     | 0.77              |
| 1:A:262:ASN:ND2  | 1:A:316:TYR:H    | 1.81                     | 0.77              |
| 2:D:170:PHE:C    | 2:D:193:SER:HB3  | 2.09                     | 0.77              |
| 1:A:504:ASN:ND2  | 1:A:507:GLN:HE21 | 1.81                     | 0.77              |
| 2:C:50:LEU:HD21  | 2:C:197:ILE:HG13 | 1.65                     | 0.77              |
| 1:A:867:LYS:HE2  | 1:A:889:ARG:HH22 | 1.48                     | 0.77              |
| 1:B:81:THR:HB    | 1:B:85:ASN:H     | 1.50                     | 0.77              |
| 2:C:208:CYS:SG   | 2:C:211:CYS:N    | 2.58                     | 0.77              |
| 1:A:909:ILE:HG12 | 1:A:928:ARG:HD2  | 1.67                     | 0.76              |
| 1:B:255:GLN:H    | 1:B:255:GLN:NE2  | 1.82                     | 0.76              |
| 2:D:15:LYS:HD2   | 2:D:41:ASN:ND2   | 1.99                     | 0.76              |
| 1:A:589:ARG:HG3  | 1:A:635:PRO:HB2  | 1.67                     | 0.76              |
| 1:B:23:PHE:N     | 1:B:30:ASN:HD22  | 1.82                     | 0.76              |
| 1:B:450:GLY:CA   | 1:B:479:VAL:CG1  | 2.64                     | 0.76              |
| 2:D:15:LYS:HD2   | 2:D:41:ASN:HD22  | 1.48                     | 0.76              |
| 1:A:901:THR:HG22 | 1:A:902:GLU:O    | 1.85                     | 0.76              |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CB   | 1.98                     | 0.76              |
| 1:A:234:GLN:HE22 | 1:A:257:THR:HA   | 1.51                     | 0.76              |
| 1:A:273:LEU:HB2  | 1:A:281:PHE:HB2  | 1.67                     | 0.76              |
| 2:D:170:PHE:O    | 2:D:193:SER:CB   | 2.30                     | 0.76              |
| 1:A:415:SER:HB3  | 1:A:423:ASP:OD1  | 1.86                     | 0.76              |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CD   | 2.10                     | 0.76              |
| 1:B:466:GLN:H    | 1:B:466:GLN:HE21 | 1.34                     | 0.76              |
| 1:B:492:GLU:HG3  | 1:B:512:VAL:HG11 | 1.68                     | 0.76              |
| 1:B:286:GLU:HB2  | 1:B:299:ASP:N    | 1.96                     | 0.76              |
| 1:A:910:MET:CE   | 1:A:912:LEU:HD21 | 2.16                     | 0.76              |
| 1:B:396:ILE:HD11 | 1:B:673:LEU:HD11 | 1.66                     | 0.75              |
| 1:B:478:LEU:HB2  | 1:B:526:LEU:HD21 | 1.68                     | 0.75              |
| 2:D:122:LEU:HD12 | 2:D:122:LEU:H    | 1.50                     | 0.75              |
| 1:A:371:GLY:HA3  | 1:A:1016:ASN:ND2 | 1.95                     | 0.75              |
| 1:B:742:VAL:HG22 | 1:B:750:THR:HG22 | 1.66                     | 0.75              |
| 1:B:405:PRO:HA   | 1:B:697:SER:HA   | 1.68                     | 0.75              |
| 1:A:184:ASP:HB2  | 1:A:185:PRO:CD   | 2.15                     | 0.75              |
| 2:D:82:LYS:C     | 2:D:83:ILE:HD12  | 2.12                     | 0.75              |
| 2:D:98:ILE:HB    | 2:D:201:ALA:HB1  | 1.68                     | 0.75              |
| 1:B:191:LYS:HG2  | 1:B:192:THR:N    | 2.02                     | 0.75              |
| 1:A:16:ASN:HD22  | 1:A:35:LYS:C     | 1.94                     | 0.75              |
| 1:B:594:THR:HG22 | 1:B:595:THR:N    | 2.02                     | 0.75              |
| 1:A:910:MET:HE3  | 1:A:912:LEU:HD21 | 1.69                     | 0.74              |
| 1:B:803:HIS:CD2  | 1:B:804:ALA:H    | 2.05                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:50:LEU:O      | 2:D:52:THR:HG23   | 1.86                     | 0.74              |
| 1:A:289:GLU:C     | 1:A:290:GLN:O     | 2.30                     | 0.74              |
| 1:B:235:GLU:H     | 1:B:253:ILE:HG22  | 1.52                     | 0.74              |
| 1:B:367:LEU:HD12  | 1:B:368:GLU:CG    | 2.17                     | 0.74              |
| 1:A:342:GLU:HG2   | 1:A:343:GLN:HG3   | 1.68                     | 0.74              |
| 1:A:798:THR:OG1   | 1:A:800:GLU:HG2   | 1.88                     | 0.74              |
| 1:B:159:LEU:HD23  | 1:B:161:GLU:H     | 1.52                     | 0.74              |
| 1:B:864:LYS:HE2   | 1:B:891:TYR:HE2   | 1.52                     | 0.74              |
| 1:B:663:ASN:HB2   | 1:B:1134:GLU:HG3  | 1.69                     | 0.74              |
| 1:A:931:LEU:HD23  | 1:A:932:LEU:N     | 2.03                     | 0.74              |
| 1:A:1032:THR:HG22 | 1:A:1036:MET:H    | 1.53                     | 0.74              |
| 1:B:1070:HIS:CE1  | 1:B:1093:LEU:HD12 | 2.23                     | 0.73              |
| 2:D:208:CYS:O     | 2:D:210:GLN:N     | 2.21                     | 0.73              |
| 1:A:750:THR:HG22  | 1:A:751:ALA:H     | 1.52                     | 0.73              |
| 1:A:903:CYS:SG    | 1:A:941:ASN:HA    | 2.28                     | 0.73              |
| 1:A:282:MET:HG2   | 1:A:305:LEU:HD11  | 1.69                     | 0.73              |
| 1:A:642:ARG:HG2   | 1:A:647:THR:HB    | 1.69                     | 0.73              |
| 1:B:368:GLU:OE2   | 1:B:391:ARG:CZ    | 2.36                     | 0.73              |
| 1:A:855:ASP:O     | 1:A:857:LYS:N     | 2.21                     | 0.73              |
| 1:B:314:LEU:O     | 1:B:314:LEU:HD12  | 1.88                     | 0.73              |
| 1:A:803:HIS:CD2   | 1:A:858:LEU:HB2   | 2.24                     | 0.73              |
| 1:B:267:ASN:ND2   | 1:B:269:SER:HB2   | 2.03                     | 0.73              |
| 2:D:108:THR:HB    | 2:D:109:PRO:HD3   | 1.71                     | 0.73              |
| 1:B:407:ILE:HD12  | 1:B:407:ILE:H     | 1.52                     | 0.73              |
| 2:D:102:LEU:HD11  | 2:D:180:VAL:HG22  | 1.70                     | 0.73              |
| 1:A:936:LYS:HE2   | 1:A:943:GLU:OE2   | 1.89                     | 0.72              |
| 1:A:873:MET:HE2   | 1:A:880:LEU:HD11  | 1.72                     | 0.72              |
| 1:B:707:ILE:CG2   | 1:B:709:LYS:HE3   | 2.20                     | 0.72              |
| 1:B:450:GLY:CA    | 1:B:479:VAL:HG13  | 2.19                     | 0.72              |
| 1:B:368:GLU:OE2   | 1:B:374:GLN:OE1   | 2.07                     | 0.72              |
| 2:C:109:PRO:HG2   | 2:C:203:ARG:NH2   | 2.03                     | 0.72              |
| 1:B:597:GLU:HG2   | 1:B:664:HIS:CE1   | 2.24                     | 0.72              |
| 2:C:52:THR:HG21   | 2:C:85:ILE:CB     | 2.19                     | 0.72              |
| 1:B:129:ARG:NH1   | 1:B:176:PRO:HD3   | 2.04                     | 0.72              |
| 1:B:130:MET:HE2   | 1:B:142:VAL:HG13  | 1.71                     | 0.71              |
| 2:D:19:THR:HG22   | 2:D:20:GLY:H      | 1.55                     | 0.71              |
| 1:A:59:GLY:HA2    | 1:A:1073:TRP:CZ3  | 2.25                     | 0.71              |
| 1:A:564:ILE:HG22  | 1:A:582:LEU:HD12  | 1.72                     | 0.71              |
| 1:A:839:GLU:CD    | 1:A:839:GLU:H     | 1.99                     | 0.71              |
| 1:B:141:LYS:HD2   | 1:B:156:ASN:OD1   | 1.90                     | 0.71              |
| 1:B:147:ARG:HE    | 1:B:147:ARG:HA    | 1.56                     | 0.71              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:451:PHE:CD2   | 1:B:451:PHE:O    | 2.43                     | 0.71              |
| 1:B:504:ASN:HD21  | 1:B:507:GLN:HB2  | 1.55                     | 0.71              |
| 2:C:30:GLN:HE21   | 2:C:36:SER:HA    | 1.54                     | 0.71              |
| 1:B:634:GLN:HB3   | 1:B:635:PRO:HD2  | 1.72                     | 0.71              |
| 1:B:246:LEU:HD13  | 1:B:300:LEU:HD13 | 1.71                     | 0.71              |
| 1:A:867:LYS:CE    | 1:A:889:ARG:HH22 | 2.04                     | 0.71              |
| 1:B:355:ASN:C     | 1:B:357:GLY:H    | 1.96                     | 0.71              |
| 1:B:23:PHE:H      | 1:B:30:ASN:ND2   | 1.83                     | 0.71              |
| 1:B:456:GLN:HE22  | 1:B:473:SER:CB   | 2.04                     | 0.71              |
| 1:A:648:ASN:HD22  | 1:A:660:TYR:HB3  | 1.56                     | 0.71              |
| 2:C:50:LEU:HD21   | 2:C:197:ILE:CG1  | 2.21                     | 0.70              |
| 1:A:750:THR:HG22  | 1:A:751:ALA:N    | 2.06                     | 0.70              |
| 1:B:124:ILE:HG23  | 1:B:131:ILE:HD13 | 1.71                     | 0.70              |
| 1:B:731:GLN:HA    | 1:B:796:GLN:HE21 | 1.56                     | 0.70              |
| 1:A:1032:THR:HG21 | 1:A:1036:MET:HB3 | 1.71                     | 0.70              |
| 1:B:643:SER:HB3   | 1:B:706:GLU:HG3  | 1.73                     | 0.70              |
| 1:B:690:SER:C     | 1:B:691:LEU:HD12 | 2.15                     | 0.70              |
| 1:A:291:MET:HG3   | 1:A:292:ASP:H    | 1.57                     | 0.70              |
| 1:A:879:LYS:HE2   | 1:A:902:GLU:OE2  | 1.91                     | 0.70              |
| 1:B:275:ASP:CG    | 1:B:279:ARG:HB2  | 2.16                     | 0.70              |
| 2:C:52:THR:CG2    | 2:C:85:ILE:HG12  | 2.20                     | 0.70              |
| 1:B:656:PRO:HB2   | 1:B:671:VAL:HB   | 1.74                     | 0.70              |
| 1:B:665:LYS:HD3   | 1:B:1138:ARG:NH1 | 2.07                     | 0.70              |
| 2:C:108:THR:O     | 2:C:110:SER:N    | 2.24                     | 0.70              |
| 2:C:164:GLY:O     | 2:C:194:CYS:HA   | 1.91                     | 0.70              |
| 2:D:99:PRO:HG2    | 2:D:106:ASP:HA   | 1.73                     | 0.70              |
| 1:B:196:SER:OG    | 1:B:199:GLU:HG2  | 1.92                     | 0.70              |
| 1:A:611:LEU:C     | 1:A:611:LEU:HD23 | 2.17                     | 0.69              |
| 1:B:63:VAL:HB     | 1:B:80:LEU:HB3   | 1.72                     | 0.69              |
| 2:D:171:HIS:CD2   | 2:D:212:PRO:HG2  | 2.25                     | 0.69              |
| 1:A:369:ARG:O     | 1:A:370:GLN:HB3  | 1.92                     | 0.69              |
| 1:B:419:ARG:NH1   | 1:B:423:ASP:HB3  | 2.05                     | 0.69              |
| 1:B:1036:MET:O    | 1:B:1037:ILE:HB  | 1.92                     | 0.69              |
| 2:C:215:CYS:SG    | 2:C:218:CYS:N    | 2.64                     | 0.69              |
| 1:A:1022:THR:HG22 | 1:A:1024:THR:H   | 1.58                     | 0.69              |
| 2:C:52:THR:CB     | 2:C:85:ILE:HA    | 2.21                     | 0.69              |
| 1:A:298:LYS:HD3   | 1:A:299:ASP:HB2  | 1.74                     | 0.69              |
| 1:A:480:SER:HB3   | 1:A:487:VAL:HG11 | 1.74                     | 0.69              |
| 1:B:107:ASN:OD1   | 1:B:109:GLN:HG2  | 1.91                     | 0.69              |
| 1:B:482:GLU:CB    | 1:B:483:PRO:HD3  | 2.18                     | 0.69              |
| 1:A:253:ILE:O     | 1:A:255:GLN:N    | 2.25                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:482:GLU:HB2  | 1:A:483:PRO:HD3   | 1.75                     | 0.69              |
| 1:A:507:GLN:NE2  | 1:A:553:SER:H     | 1.90                     | 0.69              |
| 1:B:130:MET:HG2  | 1:B:197:LEU:HD21  | 1.73                     | 0.69              |
| 1:B:369:ARG:HH12 | 1:B:670:ASN:HB3   | 1.58                     | 0.69              |
| 1:B:456:GLN:OE1  | 1:B:473:SER:HB3   | 1.93                     | 0.69              |
| 1:B:480:SER:HB3  | 1:B:485:ALA:N     | 2.08                     | 0.69              |
| 2:C:108:THR:O    | 2:C:222:THR:HA    | 1.93                     | 0.69              |
| 1:B:1026:GLY:O   | 1:B:1041:THR:HG22 | 1.92                     | 0.69              |
| 2:C:145:ILE:HD11 | 2:C:174:GLU:CD    | 2.18                     | 0.69              |
| 1:A:312:GLU:HG3  | 1:A:327:ARG:HB2   | 1.74                     | 0.68              |
| 1:B:464:ALA:O    | 1:B:465:HIS:ND1   | 2.27                     | 0.68              |
| 1:B:736:LEU:HD13 | 1:B:813:ALA:HB1   | 1.75                     | 0.68              |
| 1:A:81:THR:CG2   | 1:A:83:LYS:H      | 2.02                     | 0.68              |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CA    | 2.23                     | 0.68              |
| 1:B:449:MET:HA   | 1:B:449:MET:CE    | 2.21                     | 0.68              |
| 2:C:86:VAL:CG1   | 2:C:198:THR:HA    | 2.23                     | 0.68              |
| 1:A:844:LYS:HG3  | 1:A:845:GLN:HG3   | 1.76                     | 0.68              |
| 1:B:910:MET:HB2  | 1:B:926:LEU:HB3   | 1.75                     | 0.68              |
| 1:B:474:ALA:CB   | 1:B:477:ARG:HH22  | 1.96                     | 0.68              |
| 1:A:372:GLN:HB3  | 1:A:1014:MET:SD   | 2.34                     | 0.68              |
| 1:B:167:VAL:O    | 1:B:168:LYS:HB2   | 1.92                     | 0.68              |
| 1:A:977:CYS:HB3  | 1:A:992:LEU:HD13  | 1.75                     | 0.68              |
| 1:B:582:LEU:HD12 | 1:B:582:LEU:O     | 1.93                     | 0.68              |
| 2:C:161:PHE:CE1  | 2:C:163:ARG:HB2   | 2.29                     | 0.67              |
| 1:B:402:ILE:HD12 | 1:B:402:ILE:N     | 2.10                     | 0.67              |
| 2:D:163:ARG:H    | 2:D:163:ARG:HD2   | 1.58                     | 0.67              |
| 1:B:112:ILE:HG22 | 1:B:113:GLY:H     | 1.58                     | 0.67              |
| 1:B:450:GLY:HA2  | 1:B:479:VAL:HG13  | 1.75                     | 0.67              |
| 1:B:475:SER:HA   | 1:B:498:ILE:HD11  | 1.74                     | 0.67              |
| 1:A:706:GLU:C    | 1:A:707:ILE:HG13  | 2.19                     | 0.67              |
| 1:A:929:SER:HB3  | 1:A:952:ASN:HB2   | 1.76                     | 0.67              |
| 2:C:38:LEU:O     | 2:C:40:LYS:N      | 2.27                     | 0.67              |
| 1:A:992:LEU:HD12 | 1:A:992:LEU:O     | 1.94                     | 0.67              |
| 2:C:161:PHE:HE1  | 2:C:163:ARG:HB2   | 1.60                     | 0.67              |
| 1:A:663:ASN:O    | 1:A:664:HIS:HB2   | 1.95                     | 0.67              |
| 1:B:514:ARG:O    | 1:B:514:ARG:HG2   | 1.94                     | 0.67              |
| 2:C:88:ALA:HA    | 2:C:199:ALA:HB3   | 1.76                     | 0.67              |
| 2:D:171:HIS:HB2  | 2:D:215:CYS:HB2   | 1.76                     | 0.67              |
| 1:B:704:ILE:HD13 | 1:B:704:ILE:H     | 1.60                     | 0.66              |
| 1:B:80:LEU:HD22  | 1:B:133:LEU:HD23  | 1.76                     | 0.66              |
| 2:D:51:LEU:HD12  | 2:D:142:THR:H     | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:208:CYS:C     | 2:D:210:GLN:H     | 2.03                     | 0.66              |
| 1:A:207:TRP:HB3   | 1:A:242:GLY:HA2   | 1.77                     | 0.66              |
| 1:A:275:ASP:HB3   | 1:A:279:ARG:H     | 1.60                     | 0.66              |
| 1:A:1128:ASP:O    | 1:A:1132:VAL:HG23 | 1.94                     | 0.66              |
| 1:A:388:ARG:HD3   | 1:A:714:THR:HB    | 1.76                     | 0.66              |
| 1:A:416:ASP:HB3   | 1:A:419:ARG:CG    | 2.25                     | 0.66              |
| 1:A:23:PHE:N      | 1:A:30:ASN:HD22   | 1.84                     | 0.66              |
| 1:B:1017:LEU:HD12 | 1:B:1019:GLU:OE2  | 1.96                     | 0.66              |
| 1:B:232:ILE:CG2   | 1:B:258:ILE:HD12  | 2.25                     | 0.66              |
| 2:D:113:THR:HB    | 2:D:186:VAL:HB    | 1.78                     | 0.66              |
| 1:B:270:ARG:HG2   | 1:B:284:LEU:HD23  | 1.78                     | 0.66              |
| 1:B:743:GLN:HE21  | 1:B:782:PHE:HA    | 1.60                     | 0.66              |
| 2:D:168:GLY:CA    | 2:D:208:CYS:SG    | 2.84                     | 0.66              |
| 1:A:57:MET:HE3    | 1:A:1065:VAL:HG12 | 1.78                     | 0.66              |
| 1:B:973:ASN:HD21  | 1:B:1077:HIS:H    | 1.42                     | 0.66              |
| 1:B:1112:LEU:HD23 | 1:B:1113:GLN:N    | 2.11                     | 0.66              |
| 2:D:111:THR:C     | 2:D:188:GLU:OE2   | 2.38                     | 0.66              |
| 1:A:207:TRP:CB    | 1:A:242:GLY:HA2   | 2.27                     | 0.65              |
| 1:B:742:VAL:HG23  | 1:B:750:THR:CB    | 2.25                     | 0.65              |
| 1:B:695:ASN:HB2   | 1:B:698:THR:HG22  | 1.77                     | 0.65              |
| 1:B:707:ILE:HG23  | 1:B:709:LYS:HE3   | 1.78                     | 0.65              |
| 1:A:648:ASN:HD22  | 1:A:660:TYR:CB    | 2.09                     | 0.65              |
| 2:C:160:ASP:CG    | 2:C:161:PHE:H     | 2.04                     | 0.65              |
| 1:A:396:ILE:H     | 1:A:396:ILE:CD1   | 2.09                     | 0.65              |
| 1:B:465:HIS:CE1   | 1:B:523:PRO:HD3   | 2.32                     | 0.65              |
| 2:D:163:ARG:HD2   | 2:D:197:ILE:HD11  | 1.78                     | 0.65              |
| 1:B:1032:THR:HG22 | 1:B:1033:VAL:N    | 2.10                     | 0.65              |
| 1:A:1085:ALA:O    | 1:A:1086:THR:HG23 | 1.96                     | 0.65              |
| 1:A:1113:GLN:HB3  | 1:A:1121:LYS:HD2  | 1.78                     | 0.65              |
| 1:B:432:GLN:OE1   | 1:B:454:ASP:C     | 2.39                     | 0.65              |
| 2:D:49:GLY:HA3    | 2:D:83:ILE:HG13   | 1.79                     | 0.65              |
| 2:D:168:GLY:HA2   | 2:D:208:CYS:SG    | 2.37                     | 0.65              |
| 2:D:171:HIS:HB2   | 2:D:215:CYS:HB3   | 1.79                     | 0.65              |
| 1:A:10:GLN:HB2    | 1:A:1037:ILE:HB   | 1.78                     | 0.65              |
| 1:A:699:LEU:HD13  | 1:A:700:THR:H     | 1.58                     | 0.64              |
| 1:B:112:ILE:N     | 1:B:112:ILE:HD12  | 2.12                     | 0.64              |
| 1:B:365:VAL:O     | 1:B:367:LEU:HD23  | 1.98                     | 0.64              |
| 2:D:163:ARG:CD    | 2:D:197:ILE:HD11  | 2.26                     | 0.64              |
| 1:B:294:THR:HG22  | 1:B:295:VAL:N     | 2.05                     | 0.64              |
| 1:B:385:GLY:HA3   | 1:B:719:GLU:O     | 1.97                     | 0.64              |
| 1:B:894:THR:HG22  | 1:B:895:THR:N     | 2.11                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:564:ILE:HG22  | 1:A:564:ILE:O     | 1.97                     | 0.64              |
| 1:B:16:ASN:ND2    | 1:B:35:LYS:O      | 2.23                     | 0.64              |
| 1:B:427:LEU:HD13  | 1:B:429:PHE:HE1   | 1.62                     | 0.64              |
| 1:B:1058:LEU:HD23 | 1:B:1093:LEU:HD22 | 1.80                     | 0.64              |
| 1:B:407:ILE:HD12  | 1:B:407:ILE:N     | 2.11                     | 0.64              |
| 1:B:451:PHE:C     | 1:B:451:PHE:HD2   | 2.05                     | 0.64              |
| 1:A:368:GLU:HB3   | 1:A:370:GLN:HE22  | 1.62                     | 0.64              |
| 1:A:275:ASP:HB2   | 1:A:279:ARG:HB2   | 1.79                     | 0.64              |
| 1:B:208:LYS:HG3   | 1:B:209:GLN:H     | 1.62                     | 0.64              |
| 1:B:238:THR:HA    | 1:B:247:ALA:HA    | 1.79                     | 0.64              |
| 2:D:46:GLY:O      | 2:D:146:GLU:HG3   | 1.97                     | 0.64              |
| 1:A:492:GLU:CD    | 1:A:494:GLN:H     | 2.05                     | 0.64              |
| 1:B:432:GLN:OE1   | 1:B:454:ASP:O     | 2.16                     | 0.64              |
| 1:B:451:PHE:O     | 1:B:451:PHE:HD2   | 1.81                     | 0.64              |
| 1:B:317:LEU:O     | 1:B:318:ASP:HB2   | 1.96                     | 0.64              |
| 1:B:419:ARG:HD3   | 1:B:421:THR:O     | 1.97                     | 0.64              |
| 2:D:192:PRO:C     | 2:D:194:CYS:H     | 2.05                     | 0.64              |
| 2:D:170:PHE:N     | 2:D:170:PHE:CD1   | 2.66                     | 0.64              |
| 1:A:1051:LEU:HD22 | 1:A:1094:ILE:HG12 | 1.79                     | 0.63              |
| 1:B:19:VAL:HG22   | 1:B:20:THR:H      | 1.63                     | 0.63              |
| 1:B:682:LEU:HD13  | 1:B:683:ASN:N     | 2.13                     | 0.63              |
| 1:B:1105:MET:HE1  | 1:B:1130:ILE:HD11 | 1.81                     | 0.63              |
| 1:A:1118:SER:C    | 1:A:1120:MET:H    | 2.07                     | 0.63              |
| 1:B:272:LEU:HD22  | 1:B:280:LEU:HD11  | 1.80                     | 0.63              |
| 1:B:367:LEU:HD22  | 1:B:374:GLN:NE2   | 2.13                     | 0.63              |
| 2:D:218:CYS:HB2   | 2:D:221:ASP:OD1   | 1.98                     | 0.63              |
| 1:A:767:SER:O     | 1:A:769:LYS:HE3   | 1.98                     | 0.63              |
| 1:B:456:GLN:CD    | 1:B:473:SER:CB    | 2.64                     | 0.63              |
| 1:B:218:MET:HE2   | 1:B:218:MET:HA    | 1.79                     | 0.63              |
| 1:B:394:ILE:HD12  | 1:B:658:VAL:HB    | 1.81                     | 0.63              |
| 1:B:1022:THR:HG22 | 1:B:1024:THR:OG1  | 1.99                     | 0.63              |
| 1:B:1130:ILE:O    | 1:B:1134:GLU:HB2  | 1.97                     | 0.63              |
| 1:A:298:LYS:HD3   | 1:A:298:LYS:C     | 2.24                     | 0.63              |
| 1:B:369:ARG:HH21  | 1:B:372:GLN:CD    | 2.06                     | 0.63              |
| 1:B:866:VAL:HG12  | 1:B:884:ILE:HG21  | 1.80                     | 0.63              |
| 1:B:129:ARG:HD3   | 1:B:176:PRO:HG3   | 1.81                     | 0.63              |
| 1:B:432:GLN:O     | 1:B:433:THR:OG1   | 2.17                     | 0.63              |
| 1:B:481:GLN:NE2   | 1:B:484:LYS:NZ    | 2.47                     | 0.63              |
| 1:B:742:VAL:CG2   | 1:B:750:THR:HG22  | 2.19                     | 0.62              |
| 1:A:580:GLU:HG2   | 1:A:614:PHE:CZ    | 2.33                     | 0.62              |
| 1:A:268:GLY:O     | 1:A:270:ARG:N     | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:780:THR:HB   | 1:A:784:GLU:HB2  | 1.81                     | 0.62              |
| 1:B:368:GLU:CD   | 1:B:391:ARG:HH21 | 2.06                     | 0.62              |
| 1:B:507:GLN:NE2  | 1:B:553:SER:H    | 1.96                     | 0.62              |
| 2:D:128:LYS:HE2  | 2:D:146:GLU:OE1  | 2.00                     | 0.62              |
| 1:B:513:GLY:O    | 1:B:514:ARG:HB3  | 1.99                     | 0.62              |
| 1:B:926:LEU:HG   | 1:B:927:MET:HG3  | 1.81                     | 0.62              |
| 2:D:102:LEU:HD23 | 2:D:102:LEU:O    | 1.99                     | 0.62              |
| 1:A:986:ASP:HB2  | 1:B:1118:SER:HB3 | 1.81                     | 0.62              |
| 1:A:1114:TYR:HB2 | 1:A:1124:ALA:HB2 | 1.82                     | 0.62              |
| 1:B:803:HIS:CD2  | 1:B:804:ALA:N    | 2.67                     | 0.62              |
| 1:B:1065:VAL:C   | 1:B:1067:LYS:H   | 2.07                     | 0.62              |
| 1:B:1051:LEU:HA  | 1:B:1054:MET:HB2 | 1.80                     | 0.62              |
| 1:B:414:ARG:HB2  | 1:B:462:ASN:ND2  | 2.13                     | 0.62              |
| 1:B:456:GLN:NE2  | 1:B:473:SER:HB3  | 2.00                     | 0.62              |
| 1:B:1102:ARG:HD2 | 1:B:1105:MET:HE2 | 1.81                     | 0.62              |
| 2:C:164:GLY:HA2  | 2:C:194:CYS:O    | 2.00                     | 0.62              |
| 2:D:173:ARG:NH1  | 2:D:218:CYS:HB3  | 2.14                     | 0.62              |
| 1:A:414:ARG:HG2  | 1:A:414:ARG:HH11 | 1.64                     | 0.61              |
| 1:B:739:ARG:NH1  | 1:B:758:THR:HG23 | 2.15                     | 0.61              |
| 1:B:918:GLY:O    | 1:B:919:ASP:HB2  | 1.99                     | 0.61              |
| 1:B:474:ALA:O    | 1:B:475:SER:HB3  | 2.00                     | 0.61              |
| 1:B:629:VAL:HA   | 1:B:1017:LEU:O   | 1.99                     | 0.61              |
| 1:B:769:LYS:H    | 1:B:769:LYS:HD2  | 1.65                     | 0.61              |
| 2:D:47:VAL:HG12  | 2:D:48:THR:N     | 2.15                     | 0.61              |
| 1:B:386:SER:HA   | 1:B:717:LEU:HG   | 1.81                     | 0.61              |
| 1:B:440:GLY:O    | 1:B:686:GLY:HA3  | 2.00                     | 0.61              |
| 1:A:986:ASP:H    | 1:B:1118:SER:HB3 | 1.65                     | 0.61              |
| 1:B:14:ALA:HB1   | 1:B:327:ARG:HG3  | 1.82                     | 0.61              |
| 1:B:414:ARG:HB2  | 1:B:462:ASN:HD21 | 1.64                     | 0.61              |
| 2:C:52:THR:HG22  | 2:C:85:ILE:HG23  | 1.82                     | 0.61              |
| 1:A:16:ASN:ND2   | 1:A:35:LYS:C     | 2.56                     | 0.61              |
| 1:A:679:MET:HE2  | 1:A:691:LEU:HG   | 1.81                     | 0.61              |
| 2:C:119:GLY:O    | 2:C:120:LYS:HB2  | 1.99                     | 0.61              |
| 1:A:234:GLN:NE2  | 1:A:257:THR:HA   | 2.14                     | 0.61              |
| 1:A:358:PRO:O    | 1:A:379:SER:HA   | 2.01                     | 0.61              |
| 1:B:286:GLU:O    | 1:B:297:LEU:HD12 | 2.00                     | 0.61              |
| 1:B:644:LEU:HD23 | 1:B:644:LEU:H    | 1.66                     | 0.61              |
| 1:B:740:ILE:N    | 1:B:740:ILE:HD12 | 2.16                     | 0.61              |
| 1:A:146:ASP:C    | 1:A:148:ASP:N    | 2.56                     | 0.60              |
| 1:A:564:ILE:HG22 | 1:A:582:LEU:CD1  | 2.29                     | 0.60              |
| 1:A:722:ARG:HG3  | 1:A:722:ARG:HH11 | 1.65                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:679:MET:HE3  | 1:B:691:LEU:HD23 | 1.82                     | 0.60              |
| 1:B:1013:VAL:O   | 1:B:1014:MET:HB3 | 2.01                     | 0.60              |
| 1:A:184:ASP:HB2  | 1:A:185:PRO:HD2  | 1.83                     | 0.60              |
| 1:A:889:ARG:HD2  | 1:A:901:THR:HG23 | 1.84                     | 0.60              |
| 1:B:594:THR:CG2  | 1:B:595:THR:H    | 2.12                     | 0.60              |
| 1:B:43:VAL:HG23  | 1:B:52:VAL:HG11  | 1.83                     | 0.60              |
| 1:B:232:ILE:HG12 | 1:B:237:ILE:HG23 | 1.82                     | 0.60              |
| 1:B:693:LEU:N    | 1:B:693:LEU:HD23 | 2.16                     | 0.60              |
| 1:B:994:GLU:HG3  | 1:B:995:VAL:H    | 1.66                     | 0.60              |
| 1:A:564:ILE:N    | 1:A:564:ILE:HD12 | 2.16                     | 0.60              |
| 1:A:660:TYR:CZ   | 1:A:708:GLN:OE1  | 2.50                     | 0.60              |
| 1:B:162:LEU:H    | 1:B:162:LEU:CD2  | 2.10                     | 0.60              |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:N    | 2.16                     | 0.60              |
| 1:B:498:ILE:CG2  | 1:B:512:VAL:HG22 | 2.31                     | 0.60              |
| 2:C:180:VAL:HG12 | 2:C:180:VAL:O    | 2.02                     | 0.60              |
| 1:B:570:LYS:HG2  | 1:B:575:GLU:OE1  | 2.02                     | 0.60              |
| 1:A:848:ILE:HD11 | 1:A:870:VAL:HG11 | 1.83                     | 0.60              |
| 1:B:1118:SER:O   | 1:B:1120:MET:HG3 | 2.02                     | 0.60              |
| 2:D:147:GLU:O    | 2:D:149:ARG:N    | 2.34                     | 0.60              |
| 1:A:543:ILE:O    | 1:A:543:ILE:HG13 | 2.02                     | 0.60              |
| 1:A:161:GLU:CD   | 1:A:161:GLU:H    | 2.09                     | 0.59              |
| 1:B:356:LEU:HD23 | 1:B:388:ARG:HG3  | 1.83                     | 0.59              |
| 1:B:985:THR:O    | 1:B:989:ARG:HB3  | 2.02                     | 0.59              |
| 1:B:1108:VAL:O   | 1:B:1109:VAL:HB  | 2.02                     | 0.59              |
| 1:A:160:GLU:HB3  | 1:A:161:GLU:OE2  | 2.02                     | 0.59              |
| 1:A:300:LEU:N    | 1:A:300:LEU:HD23 | 2.17                     | 0.59              |
| 1:B:5:TYR:CE2    | 1:B:7:VAL:CG2    | 2.85                     | 0.59              |
| 2:D:143:ARG:HA   | 2:D:175:TYR:O    | 2.01                     | 0.59              |
| 1:B:167:VAL:HG12 | 1:B:180:PHE:CB   | 2.26                     | 0.59              |
| 1:A:589:ARG:HG2  | 1:A:589:ARG:HH11 | 1.66                     | 0.59              |
| 1:A:867:LYS:CD   | 1:A:867:LYS:H    | 2.15                     | 0.59              |
| 1:A:931:LEU:HD23 | 1:A:931:LEU:C    | 2.27                     | 0.59              |
| 2:D:174:GLU:O    | 2:D:188:GLU:HA   | 2.03                     | 0.59              |
| 1:B:472:THR:OG1  | 1:B:477:ARG:NH2  | 2.33                     | 0.59              |
| 1:A:743:GLN:HB3  | 1:A:782:PHE:O    | 2.03                     | 0.59              |
| 1:B:1022:THR:C   | 1:B:1024:THR:H   | 2.09                     | 0.59              |
| 2:D:22:ASN:O     | 2:D:24:VAL:N     | 2.36                     | 0.59              |
| 2:D:112:GLN:HE22 | 2:D:187:THR:HG23 | 1.67                     | 0.59              |
| 1:A:20:THR:HB    | 1:A:315:THR:HG21 | 1.84                     | 0.59              |
| 1:B:449:MET:O    | 1:B:451:PHE:N    | 2.35                     | 0.59              |
| 1:B:1032:THR:CG2 | 1:B:1033:VAL:N   | 2.66                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:208:CYS:SG    | 2:C:210:GLN:CG    | 2.88                     | 0.59              |
| 1:A:36:ASN:OD1    | 1:A:60:LYS:HD2    | 2.02                     | 0.59              |
| 1:A:117:GLU:C     | 1:A:119:GLY:H     | 2.10                     | 0.59              |
| 1:A:186:GLN:NE2   | 1:A:186:GLN:N     | 2.50                     | 0.59              |
| 1:A:532:THR:HG22  | 1:A:533:GLU:N     | 2.17                     | 0.59              |
| 1:B:192:THR:OG1   | 1:B:205:GLY:HA3   | 2.02                     | 0.59              |
| 1:B:1050:LEU:C    | 1:B:1050:LEU:HD23 | 2.28                     | 0.59              |
| 1:B:1062:ILE:HD13 | 1:B:1100:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:1070:HIS:CE1  | 1:A:1093:LEU:HD12 | 2.38                     | 0.59              |
| 1:A:188:ARG:NH1   | 1:A:216:ALA:O     | 2.36                     | 0.58              |
| 1:A:507:GLN:HE22  | 1:A:553:SER:HB3   | 1.68                     | 0.58              |
| 1:A:780:THR:HG22  | 1:A:781:SER:H     | 1.68                     | 0.58              |
| 1:B:417:PRO:HG3   | 1:B:481:GLN:OE1   | 2.03                     | 0.58              |
| 2:D:112:GLN:NE2   | 2:D:187:THR:HG23  | 2.18                     | 0.58              |
| 1:A:288:GLU:HB3   | 1:A:296:THR:HG23  | 1.86                     | 0.58              |
| 1:B:466:GLN:HE21  | 1:B:466:GLN:N     | 1.99                     | 0.58              |
| 1:B:706:GLU:O     | 1:B:707:ILE:HB    | 2.03                     | 0.58              |
| 1:B:795:ASP:HB3   | 1:B:798:THR:OG1   | 2.03                     | 0.58              |
| 1:B:866:VAL:HG11  | 1:B:884:ILE:HD12  | 1.86                     | 0.58              |
| 1:B:577:LEU:O     | 1:B:578:HIS:HB2   | 2.02                     | 0.58              |
| 1:B:199:GLU:HG3   | 1:B:201:GLU:HG2   | 1.84                     | 0.58              |
| 1:A:686:GLY:C     | 1:A:688:PRO:HD3   | 2.29                     | 0.58              |
| 1:A:982:ALA:C     | 1:A:984:THR:H     | 2.11                     | 0.58              |
| 1:B:129:ARG:HD3   | 1:B:176:PRO:CG    | 2.33                     | 0.58              |
| 1:B:341:ASN:ND2   | 1:B:342:GLU:HG2   | 2.19                     | 0.58              |
| 1:B:450:GLY:O     | 1:B:451:PHE:C     | 2.44                     | 0.58              |
| 2:C:51:LEU:HD23   | 2:C:141:MET:HA    | 1.86                     | 0.58              |
| 1:A:341:ASN:CG    | 1:A:342:GLU:N     | 2.57                     | 0.58              |
| 1:B:53:LYS:HE3    | 1:B:98:ILE:HB     | 1.85                     | 0.58              |
| 1:B:356:LEU:O     | 1:B:357:GLY:O     | 2.21                     | 0.58              |
| 1:B:1014:MET:HG3  | 1:B:1015:GLN:N    | 2.17                     | 0.58              |
| 1:B:1070:HIS:NE2  | 1:B:1093:LEU:HD12 | 2.19                     | 0.58              |
| 1:A:1032:THR:HB   | 1:A:1036:MET:O    | 2.03                     | 0.58              |
| 1:B:367:LEU:HD11  | 1:B:374:GLN:OE1   | 1.95                     | 0.58              |
| 1:B:368:GLU:HG3   | 1:B:369:ARG:HG2   | 1.86                     | 0.58              |
| 2:D:172:ARG:HH21  | 2:D:191:ASN:HD22  | 1.50                     | 0.58              |
| 1:A:766:SER:HB3   | 1:A:808:LEU:HD23  | 1.85                     | 0.58              |
| 1:A:771:PHE:CE2   | 1:A:845:GLN:HB3   | 2.39                     | 0.58              |
| 1:B:310:ILE:HG21  | 1:B:328:LEU:HD12  | 1.86                     | 0.58              |
| 1:B:864:LYS:HE2   | 1:B:891:TYR:CE2   | 2.35                     | 0.58              |
| 1:B:432:GLN:CD    | 1:B:454:ASP:O     | 2.47                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:842:GLU:HG2   | 2:D:128:LYS:NZ    | 2.18                     | 0.58              |
| 1:A:578:HIS:CD2   | 1:A:623:LEU:H     | 2.22                     | 0.58              |
| 1:A:864:LYS:HE2   | 1:A:891:TYR:HE2   | 1.68                     | 0.58              |
| 1:B:143:ILE:HG12  | 1:B:154:ALA:HB2   | 1.85                     | 0.58              |
| 1:B:437:MET:HB2   | 1:B:446:THR:HG23  | 1.85                     | 0.58              |
| 1:B:910:MET:HE3   | 1:B:912:LEU:HD21  | 1.86                     | 0.58              |
| 1:A:262:ASN:HD21  | 1:A:316:TYR:H     | 1.48                     | 0.57              |
| 1:B:248:ILE:C     | 1:B:250:PRO:HD3   | 2.29                     | 0.57              |
| 1:B:294:THR:CG2   | 1:B:295:VAL:H     | 2.11                     | 0.57              |
| 2:D:108:THR:HG22  | 2:D:109:PRO:N     | 2.17                     | 0.57              |
| 1:B:1039:LEU:HD12 | 1:B:1040:VAL:H    | 1.69                     | 0.57              |
| 1:B:1118:SER:O    | 1:B:1119:GLY:C    | 2.47                     | 0.57              |
| 2:D:173:ARG:HH12  | 2:D:218:CYS:HB3   | 1.69                     | 0.57              |
| 1:B:486:LEU:HG    | 1:B:486:LEU:O     | 2.05                     | 0.57              |
| 1:B:1028:VAL:O    | 1:B:1039:LEU:HD12 | 2.05                     | 0.57              |
| 1:B:1108:VAL:HG12 | 1:B:1109:VAL:N    | 2.19                     | 0.57              |
| 2:D:108:THR:CB    | 2:D:109:PRO:HD3   | 2.34                     | 0.57              |
| 1:B:433:THR:HG22  | 1:B:433:THR:O     | 2.03                     | 0.57              |
| 1:B:450:GLY:O     | 1:B:479:VAL:CG2   | 2.49                     | 0.57              |
| 1:B:465:HIS:O     | 1:B:467:GLN:HG3   | 2.04                     | 0.57              |
| 2:D:108:THR:O     | 2:D:109:PRO:C     | 2.46                     | 0.57              |
| 1:A:117:GLU:O     | 1:A:119:GLY:N     | 2.37                     | 0.57              |
| 1:B:256:SER:HB3   | 1:B:277:GLU:OE2   | 2.04                     | 0.57              |
| 1:B:500:VAL:HB    | 1:B:511:ALA:HB3   | 1.85                     | 0.57              |
| 1:B:550:ASN:O     | 1:B:552:LEU:N     | 2.38                     | 0.57              |
| 1:B:769:LYS:HD2   | 1:B:769:LYS:N     | 2.18                     | 0.57              |
| 1:B:24:THR:N      | 1:B:30:ASN:HD21   | 1.92                     | 0.57              |
| 1:B:365:VAL:O     | 1:B:367:LEU:CD2   | 2.52                     | 0.57              |
| 1:B:504:ASN:OD1   | 1:B:507:GLN:N     | 2.31                     | 0.57              |
| 1:A:1032:THR:CG2  | 1:A:1036:MET:H    | 2.17                     | 0.57              |
| 1:B:1054:MET:HE2  | 1:B:1054:MET:HA   | 1.87                     | 0.57              |
| 1:A:507:GLN:HE22  | 1:A:553:SER:H     | 1.51                     | 0.57              |
| 1:B:743:GLN:NE2   | 1:B:781:SER:OG    | 2.30                     | 0.57              |
| 1:B:876:PHE:CE1   | 1:B:921:ILE:HD11  | 2.40                     | 0.57              |
| 1:B:1039:LEU:HD21 | 1:B:1139:ILE:HG22 | 1.87                     | 0.57              |
| 1:A:894:THR:HG22  | 1:B:585:GLU:OE1   | 2.04                     | 0.57              |
| 1:B:433:THR:HG21  | 1:B:457:THR:CB    | 2.35                     | 0.57              |
| 1:B:641:PHE:HB3   | 1:B:679:MET:HE1   | 1.86                     | 0.56              |
| 2:C:35:THR:C      | 2:C:36:SER:O      | 2.42                     | 0.56              |
| 1:A:1101:SER:HB2  | 1:A:1103:PRO:HD2  | 1.87                     | 0.56              |
| 1:B:731:GLN:CA    | 1:B:796:GLN:HE21  | 2.17                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1057:ARG:CZ   | 1:B:1112:LEU:HB2 | 2.35                     | 0.56              |
| 2:D:202:ARG:HD2   | 2:D:204:PHE:CZ   | 2.39                     | 0.56              |
| 1:A:722:ARG:HG3   | 1:A:722:ARG:NH1  | 2.19                     | 0.56              |
| 1:B:503:CYS:SG    | 1:B:508:VAL:HG22 | 2.46                     | 0.56              |
| 1:B:731:GLN:O     | 1:B:796:GLN:HG2  | 2.05                     | 0.56              |
| 1:B:744:ASP:OD2   | 1:B:747:GLY:N    | 2.37                     | 0.56              |
| 1:B:1014:MET:CG   | 1:B:1015:GLN:N   | 2.68                     | 0.56              |
| 1:A:225:PRO:HG2   | 1:A:267:ASN:HB2  | 1.87                     | 0.56              |
| 1:B:159:LEU:CD2   | 1:B:161:GLU:HB2  | 2.36                     | 0.56              |
| 1:B:334:VAL:HG12  | 1:B:349:ALA:HA   | 1.88                     | 0.56              |
| 1:B:1075:SER:HB2  | 1:B:1084:PRO:HA  | 1.88                     | 0.56              |
| 2:C:97:PRO:HA     | 2:C:202:ARG:HA   | 1.86                     | 0.56              |
| 1:A:417:PRO:CG    | 1:A:481:GLN:HB3  | 2.33                     | 0.56              |
| 1:A:476:VAL:HG13  | 1:A:490:TRP:HB3  | 1.86                     | 0.56              |
| 1:B:255:GLN:NE2   | 1:B:255:GLN:N    | 2.52                     | 0.56              |
| 1:B:261:HIS:HA    | 1:B:272:LEU:O    | 2.06                     | 0.56              |
| 1:B:275:ASP:OD1   | 1:B:279:ARG:HB2  | 2.04                     | 0.56              |
| 2:C:52:THR:HB     | 2:C:86:VAL:H     | 1.71                     | 0.56              |
| 2:D:192:PRO:C     | 2:D:194:CYS:N    | 2.62                     | 0.56              |
| 1:A:19:VAL:HG22   | 1:A:20:THR:N     | 2.21                     | 0.56              |
| 1:A:108:VAL:O     | 1:A:141:LYS:HE2  | 2.05                     | 0.56              |
| 1:A:334:VAL:HG11  | 1:A:347:VAL:HG13 | 1.88                     | 0.56              |
| 1:A:564:ILE:HD12  | 1:A:564:ILE:H    | 1.71                     | 0.56              |
| 1:B:1125:THR:HG22 | 1:B:1127:ASP:N   | 2.15                     | 0.56              |
| 2:C:215:CYS:H     | 2:C:218:CYS:HB2  | 1.70                     | 0.56              |
| 1:A:224:GLU:HB2   | 1:A:225:PRO:HD3  | 1.87                     | 0.56              |
| 1:B:178:ILE:HG23  | 1:B:193:TYR:O    | 2.03                     | 0.56              |
| 2:C:99:PRO:HG3    | 2:C:106:ASP:O    | 2.05                     | 0.56              |
| 1:B:560:LEU:HD12  | 1:B:567:ARG:HH11 | 1.71                     | 0.56              |
| 2:D:102:LEU:CD1   | 2:D:180:VAL:HG22 | 2.36                     | 0.56              |
| 2:D:169:GLY:HA2   | 2:D:211:CYS:HA   | 1.87                     | 0.56              |
| 1:A:707:ILE:HG23  | 1:A:708:GLN:HG2  | 1.87                     | 0.56              |
| 1:B:429:PHE:O     | 1:B:432:GLN:N    | 2.28                     | 0.56              |
| 1:B:511:ALA:HB2   | 1:B:541:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:589:ARG:HG3   | 1:A:635:PRO:CB   | 2.34                     | 0.56              |
| 1:A:852:GLN:HG2   | 1:A:854:SER:H    | 1.71                     | 0.56              |
| 1:B:159:LEU:HD21  | 1:B:161:GLU:HB2  | 1.87                     | 0.56              |
| 1:B:262:ASN:ND2   | 1:B:316:TYR:H    | 2.03                     | 0.56              |
| 1:B:367:LEU:CG    | 1:B:374:GLN:CG   | 2.66                     | 0.56              |
| 2:C:163:ARG:HB3   | 2:C:195:SER:O    | 2.04                     | 0.56              |
| 1:B:223:PRO:HD3   | 1:B:271:TYR:OH   | 2.05                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:662:SER:CB   | 1:B:1138:ARG:HH21 | 2.19                     | 0.55              |
| 1:B:573:SER:O    | 1:B:574:PHE:HB2   | 2.05                     | 0.55              |
| 2:C:90:ASP:OD1   | 2:C:92:THR:HB     | 2.07                     | 0.55              |
| 2:C:100:ASN:HB3  | 2:C:103:LEU:HG    | 1.87                     | 0.55              |
| 1:A:838:PRO:HD2  | 1:A:839:GLU:OE2   | 2.05                     | 0.55              |
| 1:B:626:ARG:O    | 1:B:626:ARG:HG2   | 2.06                     | 0.55              |
| 2:D:159:ILE:HG22 | 2:D:159:ILE:O     | 2.07                     | 0.55              |
| 1:A:340:SER:HB3  | 1:A:346:TYR:CE1   | 2.41                     | 0.55              |
| 1:A:537:GLU:HB3  | 1:A:561:TRP:HB2   | 1.87                     | 0.55              |
| 1:B:206:PRO:HB2  | 1:B:207:TRP:CE3   | 2.41                     | 0.55              |
| 1:B:342:GLU:C    | 1:B:344:GLY:H     | 2.15                     | 0.55              |
| 1:B:367:LEU:CG   | 1:B:374:GLN:CD    | 2.80                     | 0.55              |
| 1:B:498:ILE:HG22 | 1:B:512:VAL:HG22  | 1.88                     | 0.55              |
| 2:D:113:THR:HG22 | 2:D:114:VAL:N     | 2.21                     | 0.55              |
| 1:B:235:GLU:H    | 1:B:253:ILE:CG2   | 2.19                     | 0.55              |
| 1:B:1120:MET:O   | 1:B:1121:LYS:HB3  | 2.06                     | 0.55              |
| 2:D:51:LEU:HD12  | 2:D:142:THR:N     | 2.21                     | 0.55              |
| 2:D:87:PRO:HG3   | 2:D:91:LYS:NZ     | 2.22                     | 0.55              |
| 1:A:117:GLU:C    | 1:A:119:GLY:N     | 2.64                     | 0.55              |
| 1:A:250:PRO:HG2  | 1:A:253:ILE:HG12  | 1.89                     | 0.55              |
| 1:A:634:GLN:HG2  | 1:A:654:ASP:OD1   | 2.06                     | 0.55              |
| 1:B:235:GLU:O    | 1:B:236:SER:HB2   | 2.07                     | 0.55              |
| 1:B:389:ILE:N    | 1:B:389:ILE:HD12  | 2.22                     | 0.55              |
| 1:B:1002:GLU:HB3 | 1:B:1032:THR:HG21 | 1.88                     | 0.55              |
| 2:D:19:THR:HG22  | 2:D:20:GLY:N      | 2.19                     | 0.55              |
| 1:A:811:GLU:HB2  | 1:A:835:MET:SD    | 2.47                     | 0.55              |
| 1:A:1119:GLY:HA3 | 1:B:984:THR:HG23  | 1.89                     | 0.55              |
| 1:B:304:LEU:C    | 1:B:304:LEU:HD23  | 2.32                     | 0.55              |
| 1:B:329:GLY:HA3  | 1:B:384:GLU:CG    | 2.34                     | 0.55              |
| 1:B:413:LEU:C    | 1:B:413:LEU:HD23  | 2.32                     | 0.55              |
| 2:C:52:THR:OG1   | 2:C:85:ILE:HA     | 2.07                     | 0.55              |
| 2:D:143:ARG:HB3  | 2:D:143:ARG:NH1   | 2.22                     | 0.55              |
| 1:A:369:ARG:O    | 1:A:370:GLN:CB    | 2.54                     | 0.55              |
| 1:A:855:ASP:CG   | 1:A:856:GLY:N     | 2.65                     | 0.55              |
| 1:B:427:LEU:HD12 | 1:B:427:LEU:H     | 1.72                     | 0.55              |
| 1:B:744:ASP:OD2  | 1:B:746:SER:C     | 2.50                     | 0.55              |
| 1:B:1065:VAL:O   | 1:B:1067:LYS:N    | 2.40                     | 0.55              |
| 1:B:355:ASN:C    | 1:B:357:GLY:N     | 2.62                     | 0.55              |
| 1:B:1022:THR:C   | 1:B:1024:THR:N    | 2.65                     | 0.55              |
| 1:B:494:GLN:O    | 1:B:494:GLN:HG2   | 2.05                     | 0.54              |
| 1:B:1108:VAL:C   | 1:B:1110:ALA:H    | 2.16                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:396:ILE:HD11  | 1:B:673:LEU:CD1   | 2.37                     | 0.54              |
| 1:B:976:VAL:O     | 1:B:994:GLU:O     | 2.24                     | 0.54              |
| 1:B:1102:ARG:HB2  | 1:B:1103:PRO:HD3  | 1.88                     | 0.54              |
| 1:B:47:GLU:CD     | 1:B:47:GLU:H      | 2.14                     | 0.54              |
| 1:B:475:SER:HB2   | 1:B:490:TRP:O     | 2.08                     | 0.54              |
| 1:B:1095:GLU:HG2  | 1:B:1137:THR:HG22 | 1.89                     | 0.54              |
| 1:A:146:ASP:O     | 1:A:148:ASP:N     | 2.41                     | 0.54              |
| 1:A:969:GLU:HG2   | 1:A:970:ASN:N     | 2.23                     | 0.54              |
| 1:B:242:GLY:O     | 1:B:243:ASP:CB    | 2.56                     | 0.54              |
| 2:C:161:PHE:HZ    | 2:C:196:PRO:HA    | 1.73                     | 0.54              |
| 1:B:165:ILE:HG21  | 1:B:217:SER:HA    | 1.90                     | 0.54              |
| 1:B:477:ARG:HD2   | 1:B:489:GLU:HG3   | 1.90                     | 0.54              |
| 1:B:560:LEU:HD12  | 1:B:567:ARG:NH1   | 2.22                     | 0.54              |
| 1:B:881:LEU:HD22  | 1:B:921:ILE:HD12  | 1.88                     | 0.54              |
| 1:B:1065:VAL:HG12 | 1:B:1066:GLY:N    | 2.23                     | 0.54              |
| 2:C:95:GLY:O      | 2:C:202:ARG:HD2   | 2.07                     | 0.54              |
| 2:D:18:GLU:OE1    | 2:D:18:GLU:HA     | 2.06                     | 0.54              |
| 1:B:282:MET:HE2   | 1:B:305:LEU:HD11  | 1.89                     | 0.54              |
| 1:B:401:SER:HA    | 1:B:700:THR:HG22  | 1.89                     | 0.54              |
| 2:C:50:LEU:CD2    | 2:C:86:VAL:HG21   | 2.37                     | 0.54              |
| 2:D:170:PHE:HD1   | 2:D:170:PHE:H     | 1.56                     | 0.54              |
| 1:A:396:ILE:CD1   | 1:A:396:ILE:N     | 2.69                     | 0.54              |
| 1:A:416:ASP:CB    | 1:A:419:ARG:HG3   | 2.35                     | 0.54              |
| 1:A:665:LYS:HD3   | 1:A:1138:ARG:CZ   | 2.37                     | 0.54              |
| 1:B:430:VAL:HG13  | 1:B:456:GLN:CB    | 2.34                     | 0.54              |
| 1:B:467:GLN:CD    | 1:B:478:LEU:HD21  | 2.33                     | 0.54              |
| 2:D:102:LEU:CD1   | 2:D:180:VAL:CG2   | 2.86                     | 0.54              |
| 1:A:189:HIS:HB3   | 1:A:210:GLU:HA    | 1.90                     | 0.54              |
| 1:A:612:PHE:CE2   | 1:A:628:LYS:HD2   | 2.43                     | 0.54              |
| 1:B:182:TYR:CZ    | 1:B:189:HIS:HB2   | 2.43                     | 0.54              |
| 1:B:228:GLY:HA2   | 1:B:241:ASN:HA    | 1.90                     | 0.54              |
| 1:B:504:ASN:ND2   | 1:B:507:GLN:HB2   | 2.22                     | 0.54              |
| 1:B:516:LEU:HD13  | 1:B:534:MET:HG2   | 1.90                     | 0.54              |
| 1:B:717:LEU:HD12  | 1:B:721:PRO:HG3   | 1.90                     | 0.54              |
| 1:B:1036:MET:O    | 1:B:1037:ILE:CB   | 2.56                     | 0.54              |
| 1:B:1102:ARG:O    | 1:B:1106:GLN:HG3  | 2.08                     | 0.54              |
| 2:D:22:ASN:O      | 2:D:23:THR:C      | 2.51                     | 0.54              |
| 1:A:130:MET:HA    | 1:A:145:LEU:HD13  | 1.90                     | 0.54              |
| 1:B:224:GLU:O     | 1:B:225:PRO:C     | 2.50                     | 0.54              |
| 1:B:616:LEU:HD12  | 1:B:617:ASN:N     | 2.22                     | 0.54              |
| 1:B:866:VAL:CG1   | 1:B:884:ILE:HG21  | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1075:SER:HB2 | 1:B:1083:GLU:O   | 2.08                     | 0.54              |
| 2:C:206:CYS:SG   | 2:C:211:CYS:HB3  | 2.48                     | 0.54              |
| 2:D:17:ILE:HD11  | 2:D:139:ASN:ND2  | 2.23                     | 0.54              |
| 1:A:889:ARG:NH1  | 1:A:904:ASN:ND2  | 2.49                     | 0.53              |
| 1:B:652:CYS:HB3  | 1:B:676:VAL:O    | 2.09                     | 0.53              |
| 1:B:949:PHE:HA   | 2:D:122:LEU:HD21 | 1.89                     | 0.53              |
| 2:D:98:ILE:HB    | 2:D:201:ALA:CB   | 2.36                     | 0.53              |
| 1:A:582:LEU:O    | 1:A:583:GLY:C    | 2.51                     | 0.53              |
| 2:C:215:CYS:O    | 2:C:219:GLU:OE1  | 2.25                     | 0.53              |
| 2:D:90:ASP:O     | 2:D:91:LYS:HG3   | 2.07                     | 0.53              |
| 2:D:171:HIS:ND1  | 2:D:215:CYS:HB3  | 2.23                     | 0.53              |
| 1:B:511:ALA:HA   | 1:B:515:ALA:O    | 2.09                     | 0.53              |
| 1:B:771:PHE:CE2  | 1:B:845:GLN:HB2  | 2.43                     | 0.53              |
| 2:C:144:PHE:HB2  | 2:C:175:TYR:HB2  | 1.91                     | 0.53              |
| 2:D:50:LEU:O     | 2:D:51:LEU:C     | 2.51                     | 0.53              |
| 1:A:867:LYS:H    | 1:A:867:LYS:HD2  | 1.73                     | 0.53              |
| 1:B:564:ILE:HG22 | 1:B:582:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:354:THR:HG21 | 1:A:712:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:414:ARG:HH21 | 1:B:462:ASN:HB2  | 1.74                     | 0.53              |
| 1:A:183:GLN:HB2  | 1:A:188:ARG:HG2  | 1.90                     | 0.53              |
| 1:A:741:GLU:CD   | 1:A:750:THR:O    | 2.52                     | 0.53              |
| 1:B:19:VAL:O     | 1:B:31:LEU:HD12  | 2.08                     | 0.53              |
| 1:B:170:LEU:HD12 | 1:B:177:THR:HG22 | 1.90                     | 0.53              |
| 1:B:413:LEU:HD22 | 1:B:424:THR:HB   | 1.90                     | 0.53              |
| 1:B:644:LEU:HG   | 1:B:645:SER:N    | 2.24                     | 0.53              |
| 1:B:731:GLN:CA   | 1:B:796:GLN:NE2  | 2.71                     | 0.53              |
| 2:C:143:ARG:NH2  | 2:C:174:GLU:OE1  | 2.42                     | 0.53              |
| 2:D:89:ASP:CG    | 2:D:202:ARG:HH21 | 2.17                     | 0.53              |
| 2:D:102:LEU:HD23 | 2:D:102:LEU:C    | 2.33                     | 0.53              |
| 2:D:169:GLY:O    | 2:D:212:PRO:CG   | 2.51                     | 0.53              |
| 1:A:487:VAL:HG23 | 1:A:524:GLN:HA   | 1.91                     | 0.53              |
| 1:A:707:ILE:CG2  | 1:A:708:GLN:HG2  | 2.39                     | 0.53              |
| 1:A:725:CYS:O    | 1:A:733:PHE:HD2  | 1.92                     | 0.53              |
| 1:B:90:GLU:HB3   | 1:B:101:ILE:HG12 | 1.91                     | 0.53              |
| 1:B:586:ILE:HG21 | 1:B:608:ASP:H    | 1.72                     | 0.53              |
| 1:B:1020:THR:O   | 1:B:1021:SER:HB2 | 2.08                     | 0.53              |
| 1:A:95:GLY:C     | 1:A:97:SER:H     | 2.15                     | 0.53              |
| 1:A:23:PHE:N     | 1:A:30:ASN:ND2   | 2.48                     | 0.53              |
| 1:B:159:LEU:HD23 | 1:B:161:GLU:N    | 2.22                     | 0.53              |
| 1:B:340:SER:HB3  | 1:B:346:TYR:CD1  | 2.43                     | 0.53              |
| 1:B:731:GLN:C    | 1:B:796:GLN:HE21 | 2.17                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:369:ARG:CG   | 1:B:369:ARG:O    | 2.56                     | 0.52              |
| 1:B:476:VAL:C    | 1:B:477:ARG:HD3  | 2.34                     | 0.52              |
| 1:B:1015:GLN:O   | 1:B:1016:ASN:C   | 2.52                     | 0.52              |
| 1:B:1079:GLU:OE2 | 1:B:1079:GLU:HA  | 2.09                     | 0.52              |
| 2:C:179:TRP:O    | 2:C:180:VAL:HB   | 2.09                     | 0.52              |
| 1:B:134:ARG:NH1  | 1:B:164:VAL:HB   | 2.25                     | 0.52              |
| 1:B:369:ARG:NH1  | 1:B:670:ASN:HB3  | 2.22                     | 0.52              |
| 2:D:87:PRO:HG3   | 2:D:91:LYS:CE    | 2.39                     | 0.52              |
| 2:D:110:SER:O    | 2:D:221:ASP:HA   | 2.10                     | 0.52              |
| 2:D:169:GLY:N    | 2:D:211:CYS:SG   | 2.69                     | 0.52              |
| 1:A:275:ASP:CB   | 1:A:279:ARG:HB2  | 2.38                     | 0.52              |
| 1:A:334:VAL:CG1  | 1:A:347:VAL:HG13 | 2.39                     | 0.52              |
| 1:B:1015:GLN:O   | 1:B:1015:GLN:HG3 | 2.09                     | 0.52              |
| 2:D:202:ARG:HB3  | 2:D:204:PHE:CE1  | 2.44                     | 0.52              |
| 1:A:1030:PHE:CZ  | 1:A:1038:GLY:HA3 | 2.44                     | 0.52              |
| 1:B:162:LEU:HG   | 1:B:163:HIS:H    | 1.74                     | 0.52              |
| 2:D:143:ARG:NH2  | 2:D:174:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:449:MET:HE2  | 1:A:449:MET:HA   | 1.92                     | 0.52              |
| 1:B:29:LEU:HB3   | 1:B:44:VAL:HB    | 1.91                     | 0.52              |
| 1:B:180:PHE:CE1  | 1:B:182:TYR:HB3  | 2.45                     | 0.52              |
| 1:B:475:SER:OG   | 1:B:477:ARG:NH1  | 2.42                     | 0.52              |
| 1:B:571:LEU:HD13 | 1:B:571:LEU:C    | 2.34                     | 0.52              |
| 1:B:741:GLU:OE1  | 1:B:749:THR:HB   | 2.09                     | 0.52              |
| 1:B:973:ASN:ND2  | 1:B:1077:HIS:H   | 2.06                     | 0.52              |
| 2:D:18:GLU:O     | 2:D:42:THR:HG23  | 2.09                     | 0.52              |
| 2:D:90:ASP:CG    | 2:D:91:LYS:H     | 2.18                     | 0.52              |
| 1:A:476:VAL:CG1  | 1:A:490:TRP:HB3  | 2.40                     | 0.52              |
| 1:A:848:ILE:CD1  | 1:A:870:VAL:HG11 | 2.40                     | 0.52              |
| 2:C:86:VAL:HG13  | 2:C:87:PRO:HD2   | 1.92                     | 0.52              |
| 2:D:115:LEU:HD23 | 2:D:123:PRO:HB3  | 1.90                     | 0.52              |
| 1:A:112:ILE:HD13 | 1:A:112:ILE:N    | 2.22                     | 0.52              |
| 1:A:655:ARG:HG3  | 1:A:655:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:922:LEU:HD23 | 1:A:957:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:10:GLN:O     | 1:B:1036:MET:O   | 2.28                     | 0.52              |
| 2:C:161:PHE:O    | 2:C:162:LYS:HB2  | 2.10                     | 0.52              |
| 1:A:780:THR:HB   | 1:A:784:GLU:CB   | 2.39                     | 0.52              |
| 1:B:489:GLU:OE2  | 1:B:491:LYS:HE3  | 2.10                     | 0.52              |
| 1:A:309:SER:HA   | 1:A:384:GLU:OE2  | 2.10                     | 0.51              |
| 1:B:228:GLY:CA   | 1:B:241:ASN:HA   | 2.40                     | 0.51              |
| 1:B:237:ILE:O    | 1:B:248:ILE:HG12 | 2.09                     | 0.51              |
| 1:B:383:LYS:HG3  | 1:B:384:GLU:OE2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:109:PRO:HG2  | 2:C:203:ARG:NH1   | 2.24                     | 0.51              |
| 2:D:171:HIS:CB   | 2:D:215:CYS:HB3   | 2.40                     | 0.51              |
| 1:A:116:SER:C    | 1:A:117:GLU:O     | 2.51                     | 0.51              |
| 1:A:837:TYR:HB3  | 1:A:839:GLU:OE2   | 2.10                     | 0.51              |
| 1:B:281:PHE:CD2  | 1:B:304:LEU:HA    | 2.46                     | 0.51              |
| 1:B:769:LYS:O    | 1:B:769:LYS:HG2   | 2.11                     | 0.51              |
| 2:D:86:VAL:HG13  | 2:D:87:PRO:HD2    | 1.92                     | 0.51              |
| 2:D:104:GLY:O    | 2:D:105:LEU:HB3   | 2.11                     | 0.51              |
| 1:A:780:THR:HG22 | 1:A:781:SER:N     | 2.24                     | 0.51              |
| 1:B:5:TYR:HB2    | 1:B:1043:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:1121:LYS:O   | 1:B:1121:LYS:HG2  | 2.10                     | 0.51              |
| 1:A:57:MET:HE3   | 1:A:1065:VAL:CG1  | 2.40                     | 0.51              |
| 1:A:1114:TYR:CB  | 1:A:1124:ALA:HB2  | 2.41                     | 0.51              |
| 1:B:910:MET:HB2  | 1:B:926:LEU:CB    | 2.41                     | 0.51              |
| 2:D:21:LEU:HD22  | 2:D:26:TYR:CD1    | 2.46                     | 0.51              |
| 1:A:912:LEU:HB2  | 1:A:913:TYR:CE1   | 2.46                     | 0.51              |
| 1:B:355:ASN:OD1  | 1:B:357:GLY:N     | 2.43                     | 0.51              |
| 1:B:393:GLY:HA2  | 1:B:708:GLN:HG2   | 1.92                     | 0.51              |
| 1:B:1126:ALA:O   | 1:B:1130:ILE:HG13 | 2.10                     | 0.51              |
| 2:C:49:GLY:HA3   | 2:C:141:MET:HE1   | 1.92                     | 0.51              |
| 2:D:87:PRO:HG3   | 2:D:91:LYS:HE3    | 1.93                     | 0.51              |
| 2:D:90:ASP:CG    | 2:D:91:LYS:N      | 2.68                     | 0.51              |
| 1:B:368:GLU:O    | 1:B:369:ARG:C     | 2.53                     | 0.51              |
| 1:B:388:ARG:NE   | 1:B:714:THR:HG23  | 2.26                     | 0.51              |
| 1:B:419:ARG:HD2  | 1:B:423:ASP:OD1   | 2.11                     | 0.51              |
| 2:C:216:SER:HA   | 2:C:219:GLU:OE2   | 2.10                     | 0.51              |
| 2:D:98:ILE:HG22  | 2:D:99:PRO:O      | 2.11                     | 0.51              |
| 2:D:110:SER:N    | 2:D:221:ASP:HB3   | 2.25                     | 0.51              |
| 1:A:634:GLN:HB3  | 1:A:635:PRO:HD2   | 1.93                     | 0.51              |
| 1:B:130:MET:HA   | 1:B:145:LEU:CB    | 2.41                     | 0.51              |
| 1:B:255:GLN:HE21 | 1:B:255:GLN:N     | 2.04                     | 0.51              |
| 1:B:290:GLN:NE2  | 1:B:293:GLY:HA3   | 2.19                     | 0.51              |
| 2:C:215:CYS:SG   | 2:C:217:GLU:HB2   | 2.51                     | 0.51              |
| 2:D:171:HIS:CG   | 2:D:215:CYS:HB3   | 2.46                     | 0.51              |
| 1:B:309:SER:O    | 1:B:310:ILE:C     | 2.54                     | 0.51              |
| 2:C:100:ASN:HB3  | 2:C:103:LEU:CD1   | 2.40                     | 0.51              |
| 2:C:167:THR:O    | 2:C:193:SER:HB3   | 2.10                     | 0.51              |
| 2:D:109:PRO:HB2  | 2:D:203:ARG:NH2   | 2.25                     | 0.51              |
| 2:D:163:ARG:NH1  | 2:D:197:ILE:HD11  | 2.25                     | 0.51              |
| 1:A:537:GLU:HB3  | 1:A:561:TRP:CB    | 2.41                     | 0.51              |
| 1:A:1026:GLY:O   | 1:A:1027:SER:HB2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1101:SER:CB  | 1:A:1103:PRO:HD2 | 2.41                     | 0.51              |
| 1:B:41:ILE:O     | 1:B:52:VAL:HG22  | 2.11                     | 0.51              |
| 1:B:451:PHE:HE2  | 1:B:453:ASP:HB3  | 1.76                     | 0.51              |
| 1:B:699:LEU:C    | 1:B:699:LEU:HD13 | 2.35                     | 0.51              |
| 1:B:986:ASP:O    | 1:B:990:GLN:HB2  | 2.10                     | 0.51              |
| 2:D:82:LYS:O     | 2:D:83:ILE:HD12  | 2.10                     | 0.51              |
| 2:D:218:CYS:O    | 2:D:221:ASP:HB2  | 2.11                     | 0.51              |
| 1:B:480:SER:O    | 1:B:484:LYS:HA   | 2.11                     | 0.51              |
| 2:C:108:THR:O    | 2:C:222:THR:CA   | 2.58                     | 0.51              |
| 2:C:178:GLY:C    | 2:C:179:TRP:HE3  | 2.19                     | 0.51              |
| 1:B:230:ILE:HD13 | 1:B:239:TYR:HD1  | 1.75                     | 0.50              |
| 1:B:687:TYR:O    | 1:B:688:PRO:O    | 2.29                     | 0.50              |
| 1:A:342:GLU:C    | 1:A:344:GLY:H    | 2.20                     | 0.50              |
| 1:A:410:LEU:HD23 | 1:A:410:LEU:N    | 2.25                     | 0.50              |
| 1:B:63:VAL:HB    | 1:B:80:LEU:CB    | 2.40                     | 0.50              |
| 1:B:134:ARG:C    | 1:B:134:ARG:HD2  | 2.36                     | 0.50              |
| 1:B:161:GLU:HB3  | 1:B:182:TYR:HB2  | 1.93                     | 0.50              |
| 1:B:1065:VAL:C   | 1:B:1067:LYS:N   | 2.69                     | 0.50              |
| 2:C:97:PRO:CD    | 2:C:202:ARG:HD3  | 2.42                     | 0.50              |
| 1:A:256:SER:OG   | 1:A:277:GLU:HG3  | 2.11                     | 0.50              |
| 1:B:151:GLU:CD   | 1:B:151:GLU:N    | 2.70                     | 0.50              |
| 1:B:861:VAL:HG12 | 1:B:862:ALA:N    | 2.26                     | 0.50              |
| 2:D:89:ASP:OD1   | 2:D:90:ASP:N     | 2.45                     | 0.50              |
| 1:A:34:ALA:HB2   | 1:A:64:MET:CE    | 2.41                     | 0.50              |
| 1:B:769:LYS:N    | 1:B:769:LYS:CD   | 2.74                     | 0.50              |
| 2:C:83:ILE:O     | 2:C:84:ALA:HB3   | 2.12                     | 0.50              |
| 1:A:465:HIS:CE1  | 1:A:523:PRO:HD3  | 2.47                     | 0.50              |
| 1:A:762:SER:HB2  | 1:A:803:HIS:HA   | 1.93                     | 0.50              |
| 1:A:794:ILE:HG23 | 1:A:799:PHE:HA   | 1.92                     | 0.50              |
| 1:A:1080:ARG:HD2 | 2:C:119:GLY:HA3  | 1.93                     | 0.50              |
| 1:B:84:TYR:CG    | 1:B:109:GLN:HB3  | 2.46                     | 0.50              |
| 1:B:250:PRO:C    | 1:B:252:ILE:H    | 2.18                     | 0.50              |
| 1:B:568:ILE:O    | 1:B:569:LEU:HD23 | 2.11                     | 0.50              |
| 1:B:571:LEU:HB3  | 1:B:572:PRO:HD3  | 1.93                     | 0.50              |
| 2:D:114:VAL:HG22 | 2:D:185:LYS:CD   | 2.39                     | 0.50              |
| 2:D:165:ARG:HG2  | 2:D:165:ARG:HH11 | 1.76                     | 0.50              |
| 1:A:1118:SER:C   | 1:A:1120:MET:N   | 2.70                     | 0.50              |
| 1:B:212:VAL:HG12 | 1:B:213:GLU:N    | 2.27                     | 0.50              |
| 1:B:223:PRO:HG2  | 1:B:268:GLY:CA   | 2.42                     | 0.50              |
| 1:B:432:GLN:NE2  | 1:B:454:ASP:O    | 2.44                     | 0.50              |
| 1:B:921:ILE:HB   | 1:B:933:LEU:HB2  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:162:LYS:O     | 2:C:162:LYS:HG3  | 2.11                     | 0.50              |
| 1:B:55:VAL:HG21   | 1:B:100:ILE:HG13 | 1.93                     | 0.50              |
| 1:B:410:LEU:HA    | 1:B:426:VAL:O    | 2.11                     | 0.50              |
| 1:B:476:VAL:CG1   | 1:B:490:TRP:HB3  | 2.38                     | 0.50              |
| 1:B:724:ILE:HA    | 1:B:734:GLY:O    | 2.12                     | 0.50              |
| 2:C:108:THR:HA    | 2:C:222:THR:O    | 2.11                     | 0.50              |
| 2:C:116:ASP:OD2   | 2:C:119:GLY:O    | 2.28                     | 0.50              |
| 2:D:95:GLY:O      | 2:D:202:ARG:NH1  | 2.38                     | 0.50              |
| 2:D:116:ASP:C     | 2:D:118:SER:H    | 2.19                     | 0.50              |
| 1:A:580:GLU:HG2   | 1:A:614:PHE:CE2  | 2.47                     | 0.50              |
| 1:B:553:SER:O     | 1:B:571:LEU:HG   | 2.11                     | 0.50              |
| 1:B:969:GLU:HG2   | 1:B:970:ASN:N    | 2.26                     | 0.50              |
| 1:B:994:GLU:HG3   | 1:B:995:VAL:N    | 2.26                     | 0.50              |
| 2:C:97:PRO:HD3    | 2:C:202:ARG:HD3  | 1.94                     | 0.50              |
| 2:D:171:HIS:NE2   | 2:D:212:PRO:CG   | 2.68                     | 0.50              |
| 1:A:704:ILE:CG2   | 1:A:705:ASP:N    | 2.73                     | 0.50              |
| 1:B:133:LEU:N     | 1:B:133:LEU:HD12 | 2.26                     | 0.50              |
| 1:B:391:ARG:HG2   | 1:B:392:ASN:N    | 2.26                     | 0.50              |
| 1:A:597:GLU:OE2   | 1:A:664:HIS:N    | 2.41                     | 0.49              |
| 1:B:377:THR:O     | 1:B:387:LEU:HA   | 2.12                     | 0.49              |
| 1:B:468:LEU:HD13  | 1:B:481:GLN:HG2  | 1.94                     | 0.49              |
| 1:B:675:GLU:HG2   | 1:B:676:VAL:N    | 2.27                     | 0.49              |
| 1:B:728:GLU:C     | 1:B:730:SER:H    | 2.20                     | 0.49              |
| 2:C:52:THR:O      | 2:C:53:ASN:C     | 2.45                     | 0.49              |
| 1:B:91:TYR:OH     | 1:B:98:ILE:HD12  | 2.12                     | 0.49              |
| 2:D:169:GLY:C     | 2:D:212:PRO:HD2  | 2.24                     | 0.49              |
| 1:A:1032:THR:HG22 | 1:A:1036:MET:N   | 2.25                     | 0.49              |
| 1:B:170:LEU:HD12  | 1:B:177:THR:CG2  | 2.40                     | 0.49              |
| 1:B:790:ASN:N     | 1:B:790:ASN:ND2  | 2.58                     | 0.49              |
| 1:B:1017:LEU:C    | 1:B:1019:GLU:H   | 2.20                     | 0.49              |
| 1:B:1080:ARG:NE   | 1:B:1080:ARG:HA  | 2.28                     | 0.49              |
| 2:D:48:THR:HB     | 2:D:145:ILE:CD1  | 2.42                     | 0.49              |
| 1:A:125:ASP:OD2   | 1:A:127:GLU:HB2  | 2.12                     | 0.49              |
| 1:A:356:LEU:O     | 1:A:379:SER:HB3  | 2.12                     | 0.49              |
| 1:A:594:THR:HG23  | 1:A:595:THR:N    | 2.26                     | 0.49              |
| 1:A:1057:ARG:NH1  | 1:A:1112:LEU:HB2 | 2.28                     | 0.49              |
| 1:B:262:ASN:ND2   | 1:B:315:THR:HA   | 2.26                     | 0.49              |
| 1:B:359:ILE:HG13  | 1:B:1035:GLY:HA2 | 1.95                     | 0.49              |
| 1:B:548:ASP:O     | 1:B:550:ASN:N    | 2.45                     | 0.49              |
| 1:B:743:GLN:HB2   | 1:B:783:GLY:H    | 1.78                     | 0.49              |
| 2:C:102:LEU:C     | 2:C:104:GLY:H    | 2.21                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:546:LEU:HD11 | 1:B:593:MET:HB3  | 1.95                     | 0.49              |
| 1:B:614:PHE:N    | 1:B:614:PHE:CD1  | 2.79                     | 0.49              |
| 1:A:29:LEU:HG    | 1:A:44:VAL:HG21  | 1.94                     | 0.49              |
| 1:B:467:GLN:HB3  | 1:B:478:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:337:ASN:O    | 1:A:346:TYR:HB3  | 2.12                     | 0.49              |
| 1:A:745:THR:C    | 1:A:747:GLY:H    | 2.21                     | 0.49              |
| 1:A:794:ILE:CG2  | 1:A:799:PHE:HA   | 2.43                     | 0.49              |
| 1:B:910:MET:CE   | 1:B:912:LEU:HD21 | 2.43                     | 0.49              |
| 1:A:2:SER:HB2    | 1:A:995:VAL:CG2  | 2.42                     | 0.49              |
| 1:A:365:VAL:CG1  | 1:A:367:LEU:HG   | 2.43                     | 0.49              |
| 1:A:576:LEU:HD22 | 1:A:578:HIS:H    | 1.77                     | 0.49              |
| 1:A:1113:GLN:HA  | 1:A:1113:GLN:OE1 | 2.12                     | 0.49              |
| 1:B:226:PHE:HD2  | 1:B:297:LEU:HB2  | 1.76                     | 0.49              |
| 2:C:97:PRO:N     | 2:C:202:ARG:HD3  | 2.28                     | 0.49              |
| 2:D:103:LEU:O    | 2:D:105:LEU:HD23 | 2.12                     | 0.49              |
| 1:B:114:ARG:HG3  | 1:B:137:ASP:OD2  | 2.12                     | 0.49              |
| 1:B:257:THR:HG22 | 1:B:258:ILE:N    | 2.28                     | 0.49              |
| 1:B:358:PRO:O    | 1:B:379:SER:HA   | 2.13                     | 0.49              |
| 1:B:477:ARG:HB3  | 1:B:489:GLU:HG3  | 1.95                     | 0.49              |
| 1:B:485:ALA:O    | 1:B:487:VAL:HG13 | 2.13                     | 0.49              |
| 1:B:876:PHE:HD1  | 1:B:916:THR:HG21 | 1.78                     | 0.49              |
| 1:A:44:VAL:HG11  | 1:A:317:LEU:HB3  | 1.94                     | 0.49              |
| 1:A:564:ILE:N    | 1:A:564:ILE:CD1  | 2.75                     | 0.49              |
| 1:A:903:CYS:CB   | 1:A:941:ASN:HA   | 2.43                     | 0.49              |
| 1:B:57:MET:CE    | 1:B:1066:GLY:H   | 2.23                     | 0.49              |
| 1:B:267:ASN:HD21 | 1:B:269:SER:CB   | 2.13                     | 0.49              |
| 1:B:451:PHE:CE2  | 1:B:453:ASP:HB3  | 2.48                     | 0.49              |
| 1:B:665:LYS:HD3  | 1:B:1138:ARG:CZ  | 2.43                     | 0.49              |
| 1:B:771:PHE:HE2  | 1:B:845:GLN:HB2  | 1.76                     | 0.49              |
| 2:C:179:TRP:O    | 2:C:183:GLU:O    | 2.30                     | 0.49              |
| 1:A:446:THR:HG22 | 1:A:447:GLU:N    | 2.28                     | 0.48              |
| 1:A:657:THR:HG23 | 1:A:669:SER:O    | 2.12                     | 0.48              |
| 1:A:926:LEU:O    | 1:A:953:TRP:HA   | 2.12                     | 0.48              |
| 2:C:40:LYS:HG2   | 2:C:42:THR:HG23  | 1.95                     | 0.48              |
| 1:A:177:THR:CG2  | 1:A:194:GLU:HG2  | 2.43                     | 0.48              |
| 1:B:165:ILE:CD1  | 1:B:188:ARG:HH12 | 2.25                     | 0.48              |
| 1:B:602:LEU:C    | 1:B:602:LEU:HD13 | 2.38                     | 0.48              |
| 2:C:136:GLY:O    | 2:C:139:ASN:O    | 2.31                     | 0.48              |
| 2:D:177:ILE:HG23 | 2:D:186:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:385:GLY:HA3  | 1:A:719:GLU:O    | 2.13                     | 0.48              |
| 1:A:589:ARG:HG2  | 1:A:589:ARG:NH1  | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:594:THR:CG2  | 1:A:595:THR:N     | 2.75                     | 0.48              |
| 1:A:876:PHE:HD1  | 1:A:916:THR:HG21  | 1.78                     | 0.48              |
| 1:A:1121:LYS:HZ3 | 1:A:1121:LYS:HB2  | 1.78                     | 0.48              |
| 1:B:130:MET:HE3  | 1:B:195:VAL:HG11  | 1.96                     | 0.48              |
| 1:B:355:ASN:CG   | 1:B:357:GLY:H     | 2.21                     | 0.48              |
| 1:B:843:PRO:HD3  | 2:D:22:ASN:HD21   | 1.78                     | 0.48              |
| 1:A:95:GLY:C     | 1:A:97:SER:N      | 2.71                     | 0.48              |
| 1:A:288:GLU:HB3  | 1:A:296:THR:CG2   | 2.42                     | 0.48              |
| 1:A:413:LEU:HD23 | 1:A:462:ASN:OD1   | 2.14                     | 0.48              |
| 1:A:487:VAL:O    | 1:A:488:SER:HB2   | 2.13                     | 0.48              |
| 1:B:423:ASP:O    | 1:B:438:LEU:HB2   | 2.12                     | 0.48              |
| 1:B:437:MET:CB   | 1:B:446:THR:HG23  | 2.43                     | 0.48              |
| 1:B:612:PHE:CE2  | 1:B:628:LYS:HD2   | 2.49                     | 0.48              |
| 1:B:1047:TRP:HZ3 | 1:B:1132:VAL:HG13 | 1.79                     | 0.48              |
| 2:C:48:THR:HG23  | 2:C:82:LYS:HG2    | 1.94                     | 0.48              |
| 2:C:160:ASP:OD2  | 2:C:161:PHE:N     | 2.47                     | 0.48              |
| 2:C:192:PRO:HB3  | 2:C:206:CYS:SG    | 2.53                     | 0.48              |
| 2:D:22:ASN:C     | 2:D:22:ASN:HD22   | 2.20                     | 0.48              |
| 2:D:163:ARG:NH1  | 2:D:197:ILE:CD1   | 2.76                     | 0.48              |
| 1:A:81:THR:CG2   | 1:A:82:ALA:N      | 2.75                     | 0.48              |
| 1:A:239:TYR:CE2  | 1:A:241:ASN:HB2   | 2.48                     | 0.48              |
| 1:B:52:VAL:HG23  | 1:B:53:LYS:N      | 2.29                     | 0.48              |
| 1:B:821:LEU:O    | 1:B:822:GLY:C     | 2.57                     | 0.48              |
| 2:D:104:GLY:C    | 2:D:105:LEU:HD23  | 2.39                     | 0.48              |
| 2:D:140:LEU:N    | 2:D:140:LEU:HD23  | 2.29                     | 0.48              |
| 1:A:475:SER:HB2  | 1:A:490:TRP:O     | 2.13                     | 0.48              |
| 1:B:239:TYR:CE2  | 1:B:241:ASN:HB2   | 2.48                     | 0.48              |
| 1:B:824:ASP:OD2  | 1:B:828:TYR:OH    | 2.28                     | 0.48              |
| 1:B:896:GLU:O    | 1:B:897:LYS:HB2   | 2.12                     | 0.48              |
| 2:C:50:LEU:HD22  | 2:C:86:VAL:HG21   | 1.95                     | 0.48              |
| 2:D:173:ARG:NH1  | 2:D:190:CYS:SG    | 2.87                     | 0.48              |
| 1:B:80:LEU:CD2   | 1:B:133:LEU:HD23  | 2.43                     | 0.48              |
| 1:B:480:SER:OG   | 1:B:483:PRO:HD2   | 2.13                     | 0.48              |
| 1:B:655:ARG:HG2  | 1:B:655:ARG:HH11  | 1.77                     | 0.48              |
| 1:B:941:ASN:C    | 1:B:941:ASN:HD22  | 2.22                     | 0.48              |
| 2:D:198:THR:HG21 | 2:D:204:PHE:HZ    | 1.78                     | 0.48              |
| 1:A:401:SER:C    | 1:A:402:ILE:HD13  | 2.39                     | 0.48              |
| 1:A:542:ASP:OD1  | 1:A:593:MET:N     | 2.45                     | 0.48              |
| 1:B:356:LEU:O    | 1:B:357:GLY:C     | 2.57                     | 0.48              |
| 1:B:617:ASN:OD1  | 1:B:619:GLU:HB2   | 2.14                     | 0.48              |
| 1:B:786:VAL:HG23 | 1:B:786:VAL:O     | 2.14                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:19:THR:HA    | 2:D:43:ILE:HG23   | 1.96                     | 0.48              |
| 1:A:256:SER:HB3  | 1:A:275:ASP:CG    | 2.39                     | 0.48              |
| 1:A:318:ASP:O    | 1:A:319:ASN:C     | 2.57                     | 0.48              |
| 1:A:537:GLU:O    | 1:A:561:TRP:HB2   | 2.14                     | 0.48              |
| 1:A:954:MET:HE1  | 1:A:975:PHE:CZ    | 2.48                     | 0.48              |
| 1:B:286:GLU:HB3  | 1:B:298:LYS:HD3   | 1.95                     | 0.48              |
| 1:B:523:PRO:C    | 1:B:524:GLN:NE2   | 2.72                     | 0.48              |
| 1:B:1007:PHE:CD2 | 1:B:1030:PHE:HB3  | 2.49                     | 0.48              |
| 2:C:18:GLU:OE1   | 2:C:40:LYS:HD2    | 2.14                     | 0.48              |
| 2:D:108:THR:CB   | 2:D:109:PRO:CD    | 2.92                     | 0.48              |
| 1:B:162:LEU:HD23 | 1:B:162:LEU:N     | 2.17                     | 0.48              |
| 1:B:459:PHE:CD2  | 1:B:503:CYS:HB3   | 2.48                     | 0.48              |
| 1:B:835:MET:HB2  | 1:B:845:GLN:HG3   | 1.95                     | 0.48              |
| 2:D:115:LEU:HG   | 2:D:130:VAL:HG13  | 1.96                     | 0.48              |
| 1:A:729:VAL:HG23 | 1:A:730:SER:N     | 2.28                     | 0.47              |
| 1:A:839:GLU:CD   | 1:A:839:GLU:N     | 2.69                     | 0.47              |
| 1:B:32:LEU:HD12  | 1:B:32:LEU:N      | 2.28                     | 0.47              |
| 1:B:57:MET:HE3   | 1:B:1065:VAL:HB   | 1.95                     | 0.47              |
| 1:B:81:THR:HG22  | 1:B:83:LYS:N      | 2.06                     | 0.47              |
| 1:B:456:GLN:O    | 1:B:472:THR:HG22  | 2.14                     | 0.47              |
| 1:B:794:ILE:HG22 | 1:B:799:PHE:HA    | 1.96                     | 0.47              |
| 1:B:1014:MET:O   | 1:B:1015:GLN:HB3  | 2.14                     | 0.47              |
| 2:D:103:LEU:O    | 2:D:105:LEU:N     | 2.47                     | 0.47              |
| 1:A:1051:LEU:HB2 | 1:A:1089:ILE:HD13 | 1.95                     | 0.47              |
| 1:A:1102:ARG:N   | 1:A:1103:PRO:CD   | 2.78                     | 0.47              |
| 1:B:427:LEU:HD13 | 1:B:429:PHE:CE1   | 2.48                     | 0.47              |
| 1:B:532:THR:HB   | 1:B:574:PHE:CD1   | 2.49                     | 0.47              |
| 2:C:177:ILE:N    | 2:C:177:ILE:HD12  | 2.29                     | 0.47              |
| 1:A:112:ILE:H    | 1:A:112:ILE:CD1   | 2.20                     | 0.47              |
| 2:C:215:CYS:H    | 2:C:218:CYS:CB    | 2.27                     | 0.47              |
| 1:A:520:GLN:HG3  | 1:A:529:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:1051:LEU:CB  | 1:A:1089:ILE:HD13 | 2.44                     | 0.47              |
| 1:B:68:ARG:HB2   | 1:B:75:ASP:OD2    | 2.14                     | 0.47              |
| 1:B:199:GLU:HG3  | 1:B:201:GLU:CG    | 2.45                     | 0.47              |
| 1:B:207:TRP:CZ3  | 1:B:241:ASN:O     | 2.68                     | 0.47              |
| 1:B:458:PHE:CD1  | 1:B:458:PHE:N     | 2.82                     | 0.47              |
| 1:B:847:ARG:NH1  | 1:B:849:VAL:HG22  | 2.29                     | 0.47              |
| 1:B:991:HIS:HB3  | 1:B:993:GLN:NE2   | 2.29                     | 0.47              |
| 2:C:16:LEU:O     | 2:C:41:ASN:HB2    | 2.14                     | 0.47              |
| 2:D:21:LEU:HD22  | 2:D:26:TYR:HD1    | 1.78                     | 0.47              |
| 1:A:1:MET:HA     | 1:A:1:MET:HE2     | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:59:GLY:HA2    | 1:A:1073:TRP:CE3  | 2.48                     | 0.47              |
| 1:A:256:SER:HB3   | 1:A:275:ASP:OD1   | 2.13                     | 0.47              |
| 1:A:333:LEU:HD12  | 1:A:333:LEU:HA    | 1.75                     | 0.47              |
| 1:A:570:LYS:HG3   | 1:A:572:PRO:HD2   | 1.97                     | 0.47              |
| 1:B:242:GLY:O     | 1:B:243:ASP:HB2   | 2.14                     | 0.47              |
| 2:D:22:ASN:C      | 2:D:22:ASN:ND2    | 2.72                     | 0.47              |
| 1:A:213:GLU:OE1   | 1:A:236:SER:HB3   | 2.14                     | 0.47              |
| 1:A:634:GLN:HG2   | 1:A:654:ASP:CG    | 2.40                     | 0.47              |
| 1:B:886:SER:O     | 1:B:908:ASN:ND2   | 2.48                     | 0.47              |
| 1:B:961:ASP:C     | 1:B:961:ASP:OD2   | 2.58                     | 0.47              |
| 1:B:1048:TYR:HE2  | 1:B:1052:LEU:HD12 | 1.79                     | 0.47              |
| 1:B:1115:ASP:HB2  | 1:B:1120:MET:CB   | 2.45                     | 0.47              |
| 2:D:16:LEU:O      | 2:D:41:ASN:HB3    | 2.14                     | 0.47              |
| 1:A:364:VAL:HG21  | 1:A:1010:GLY:HA3  | 1.97                     | 0.47              |
| 1:A:367:LEU:HD12  | 1:A:374:GLN:NE2   | 2.30                     | 0.47              |
| 1:A:518:TYR:CD1   | 1:A:571:LEU:HD22  | 2.49                     | 0.47              |
| 1:A:597:GLU:HG3   | 1:A:661:SER:HB3   | 1.95                     | 0.47              |
| 1:A:889:ARG:CD    | 1:A:901:THR:HG23  | 2.44                     | 0.47              |
| 1:A:1055:GLN:HE22 | 1:A:1090:ASP:H    | 1.63                     | 0.47              |
| 1:B:147:ARG:HA    | 1:B:147:ARG:NE    | 2.26                     | 0.47              |
| 1:B:289:GLU:OE2   | 1:B:289:GLU:HA    | 2.14                     | 0.47              |
| 1:B:722:ARG:NH1   | 2:D:28:THR:HG21   | 2.30                     | 0.47              |
| 1:A:550:ASN:O     | 1:A:552:LEU:N     | 2.48                     | 0.47              |
| 1:A:867:LYS:CE    | 1:A:889:ARG:NH2   | 2.77                     | 0.47              |
| 1:A:969:GLU:OE2   | 1:A:971:ALA:HB3   | 2.14                     | 0.47              |
| 1:B:131:ILE:HB    | 1:B:143:ILE:HB    | 1.96                     | 0.47              |
| 1:B:147:ARG:O     | 1:B:148:ASP:C     | 2.58                     | 0.47              |
| 1:B:290:GLN:HG3   | 1:B:293:GLY:H     | 1.80                     | 0.47              |
| 1:B:458:PHE:N     | 1:B:458:PHE:HD1   | 2.13                     | 0.47              |
| 1:B:514:ARG:HB2   | 1:B:537:GLU:HA    | 1.96                     | 0.47              |
| 1:B:739:ARG:NH1   | 1:B:757:SER:OG    | 2.47                     | 0.47              |
| 1:B:976:VAL:HG22  | 1:B:996:GLY:CA    | 2.35                     | 0.47              |
| 1:B:1125:THR:HG22 | 1:B:1126:ALA:N    | 2.30                     | 0.47              |
| 1:A:19:VAL:HG22   | 1:A:20:THR:H      | 1.78                     | 0.47              |
| 1:A:68:ARG:HD2    | 1:A:74:LYS:C      | 2.40                     | 0.47              |
| 1:A:213:GLU:OE2   | 1:A:215:GLU:HB2   | 2.14                     | 0.47              |
| 1:A:235:GLU:O     | 1:A:249:ALA:HA    | 2.15                     | 0.47              |
| 1:A:931:LEU:C     | 1:A:931:LEU:CD2   | 2.87                     | 0.47              |
| 1:B:275:ASP:HB3   | 1:B:277:GLU:H     | 1.80                     | 0.47              |
| 2:D:47:VAL:HG12   | 2:D:48:THR:H      | 1.79                     | 0.47              |
| 2:D:108:THR:HB    | 2:D:109:PRO:CD    | 2.41                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:116:ASP:O    | 2:D:118:SER:N    | 2.45                     | 0.47              |
| 1:A:479:VAL:HG12 | 1:A:480:SER:O    | 2.15                     | 0.47              |
| 1:B:575:GLU:O    | 1:B:576:LEU:C    | 2.58                     | 0.47              |
| 1:B:832:GLY:N    | 1:B:873:MET:HE2  | 2.30                     | 0.47              |
| 1:A:110:ASP:HB2  | 1:A:136:TYR:CE1  | 2.50                     | 0.46              |
| 1:A:465:HIS:O    | 1:A:467:GLN:HG3  | 2.15                     | 0.46              |
| 1:A:741:GLU:HB3  | 1:A:750:THR:O    | 2.14                     | 0.46              |
| 1:A:870:VAL:HG22 | 1:A:884:ILE:HG13 | 1.96                     | 0.46              |
| 1:B:253:ILE:HG22 | 1:B:253:ILE:O    | 2.15                     | 0.46              |
| 1:B:390:ILE:HG22 | 1:B:710:LEU:HD22 | 1.96                     | 0.46              |
| 1:B:498:ILE:HG23 | 1:B:512:VAL:HG22 | 1.97                     | 0.46              |
| 1:B:512:VAL:O    | 1:B:513:GLY:C    | 2.57                     | 0.46              |
| 2:C:172:ARG:CZ   | 2:C:197:ILE:HG22 | 2.44                     | 0.46              |
| 1:A:465:HIS:HB2  | 1:A:467:GLN:HE21 | 1.79                     | 0.46              |
| 1:A:717:LEU:O    | 1:A:718:TYR:HB2  | 2.15                     | 0.46              |
| 1:B:124:ILE:HG23 | 1:B:131:ILE:CD1  | 2.42                     | 0.46              |
| 1:B:437:MET:HE2  | 1:B:444:GLU:HB2  | 1.97                     | 0.46              |
| 2:C:147:GLU:HG2  | 2:C:172:ARG:HG3  | 1.96                     | 0.46              |
| 1:A:360:VAL:O    | 1:A:360:VAL:HG12 | 2.16                     | 0.46              |
| 1:A:927:MET:CE   | 2:C:130:VAL:HG11 | 2.46                     | 0.46              |
| 1:B:408:LYS:CB   | 1:B:430:VAL:HG23 | 2.44                     | 0.46              |
| 1:B:436:LEU:HA   | 1:B:445:GLU:HA   | 1.97                     | 0.46              |
| 1:B:475:SER:HA   | 1:B:498:ILE:CD1  | 2.42                     | 0.46              |
| 1:B:789:HIS:ND1  | 1:B:812:TYR:HA   | 2.31                     | 0.46              |
| 2:C:161:PHE:CD1  | 2:C:197:ILE:HD12 | 2.51                     | 0.46              |
| 2:D:139:ASN:O    | 2:D:140:LEU:C    | 2.58                     | 0.46              |
| 1:A:1097:PHE:CZ  | 1:A:1105:MET:HG2 | 2.50                     | 0.46              |
| 1:A:1121:LYS:HD3 | 1:A:1122:ARG:H   | 1.81                     | 0.46              |
| 1:B:226:PHE:CD1  | 1:B:226:PHE:N    | 2.84                     | 0.46              |
| 1:B:466:GLN:H    | 1:B:466:GLN:NE2  | 2.07                     | 0.46              |
| 1:A:234:GLN:O    | 1:A:235:GLU:CG   | 2.63                     | 0.46              |
| 1:A:745:THR:HG23 | 1:A:782:PHE:CE1  | 2.51                     | 0.46              |
| 1:A:750:THR:CG2  | 1:A:751:ALA:H    | 2.17                     | 0.46              |
| 1:B:308:THR:OG1  | 1:B:309:SER:N    | 2.38                     | 0.46              |
| 1:B:450:GLY:C    | 1:B:479:VAL:CG2  | 2.89                     | 0.46              |
| 1:B:683:ASN:HA   | 1:B:688:PRO:O    | 2.14                     | 0.46              |
| 1:B:790:ASN:HA   | 1:B:807:PHE:CD1  | 2.51                     | 0.46              |
| 1:B:1105:MET:CE  | 1:B:1126:ALA:HB1 | 2.31                     | 0.46              |
| 2:D:43:ILE:HG23  | 2:D:43:ILE:O     | 2.15                     | 0.46              |
| 1:B:59:GLY:HA2   | 1:B:1073:TRP:CZ3 | 2.50                     | 0.46              |
| 1:B:63:VAL:CB    | 1:B:80:LEU:HB3   | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:314:LEU:HD12  | 1:B:314:LEU:C     | 2.40                     | 0.46              |
| 1:B:342:GLU:C     | 1:B:344:GLY:N     | 2.73                     | 0.46              |
| 1:B:518:TYR:CZ    | 1:B:571:LEU:HD11  | 2.50                     | 0.46              |
| 1:B:983:ALA:O     | 1:B:985:THR:N     | 2.44                     | 0.46              |
| 1:B:1002:GLU:HB3  | 1:B:1032:THR:CG2  | 2.45                     | 0.46              |
| 1:A:429:PHE:O     | 1:A:430:VAL:C     | 2.56                     | 0.46              |
| 1:A:587:ILE:HD13  | 1:A:587:ILE:H     | 1.80                     | 0.46              |
| 1:B:142:VAL:O     | 1:B:154:ALA:HB1   | 2.15                     | 0.46              |
| 1:B:492:GLU:O     | 1:B:493:PRO:C     | 2.59                     | 0.46              |
| 1:B:881:LEU:CD2   | 1:B:921:ILE:HD12  | 2.46                     | 0.46              |
| 1:B:984:THR:HG22  | 1:B:984:THR:O     | 2.15                     | 0.46              |
| 1:A:665:LYS:HB3   | 1:A:1138:ARG:NH2  | 2.31                     | 0.46              |
| 1:A:938:MET:HE3   | 1:B:627:LYS:HA    | 1.97                     | 0.46              |
| 1:A:1098:LEU:HD11 | 1:A:1133:VAL:HG12 | 1.97                     | 0.46              |
| 1:B:311:ALA:HB2   | 1:B:324:VAL:HG13  | 1.98                     | 0.46              |
| 1:B:414:ARG:HG2   | 1:B:414:ARG:HH11  | 1.81                     | 0.46              |
| 1:B:447:GLU:O     | 1:B:448:LEU:HD12  | 2.15                     | 0.46              |
| 1:B:548:ASP:O     | 1:B:549:SER:C     | 2.59                     | 0.46              |
| 1:B:662:SER:HB2   | 1:B:1138:ARG:HH21 | 1.79                     | 0.46              |
| 1:B:1014:MET:CG   | 1:B:1015:GLN:H    | 2.28                     | 0.46              |
| 2:D:17:ILE:O      | 2:D:17:ILE:HG22   | 2.16                     | 0.46              |
| 2:D:28:THR:HA     | 2:D:31:GLN:HE21   | 1.80                     | 0.46              |
| 2:D:52:THR:OG1    | 2:D:85:ILE:HA     | 2.15                     | 0.46              |
| 1:A:234:GLN:O     | 1:A:235:GLU:CB    | 2.64                     | 0.46              |
| 1:A:269:SER:O     | 1:A:284:LEU:HA    | 2.15                     | 0.46              |
| 1:A:594:THR:HG23  | 1:A:595:THR:H     | 1.80                     | 0.46              |
| 1:B:124:ILE:HG12  | 1:B:131:ILE:CD1   | 2.46                     | 0.46              |
| 1:B:289:GLU:OE2   | 1:B:295:VAL:HG12  | 2.16                     | 0.46              |
| 2:D:149:ARG:O     | 2:D:150:GLU:O     | 2.33                     | 0.46              |
| 2:D:171:HIS:HA    | 2:D:193:SER:H     | 1.81                     | 0.46              |
| 2:D:206:CYS:SG    | 2:D:208:CYS:O     | 2.74                     | 0.46              |
| 1:A:131:ILE:HG22  | 1:A:133:LEU:HD13  | 1.98                     | 0.45              |
| 1:A:910:MET:HE2   | 1:A:912:LEU:HD21  | 1.96                     | 0.45              |
| 1:B:905:HIS:CD2   | 1:B:933:LEU:HD21  | 2.50                     | 0.45              |
| 1:B:1048:TYR:CE2  | 1:B:1052:LEU:HD12 | 2.51                     | 0.45              |
| 2:C:160:ASP:CG    | 2:C:161:PHE:N     | 2.72                     | 0.45              |
| 2:D:142:THR:O     | 2:D:143:ARG:C     | 2.59                     | 0.45              |
| 2:D:208:CYS:O     | 2:D:208:CYS:SG    | 2.75                     | 0.45              |
| 1:A:334:VAL:HG22  | 1:A:349:ALA:HA    | 1.98                     | 0.45              |
| 1:B:412:PRO:HB2   | 1:B:422:TYR:CD2   | 2.51                     | 0.45              |
| 1:B:422:TYR:HD1   | 1:B:422:TYR:H     | 1.63                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:426:VAL:HG22  | 1:B:435:VAL:HG13  | 1.99                     | 0.45              |
| 1:B:706:GLU:O     | 1:B:707:ILE:CB    | 2.64                     | 0.45              |
| 1:B:947:ARG:C     | 1:B:992:LEU:HD12  | 2.41                     | 0.45              |
| 1:B:994:GLU:CG    | 1:B:995:VAL:H     | 2.29                     | 0.45              |
| 1:A:18:CYS:N      | 1:A:313:CYS:SG    | 2.89                     | 0.45              |
| 1:A:396:ILE:HD13  | 1:A:396:ILE:N     | 2.11                     | 0.45              |
| 1:A:576:LEU:HD22  | 1:A:578:HIS:N     | 2.31                     | 0.45              |
| 1:A:652:CYS:HB3   | 1:A:676:VAL:O     | 2.17                     | 0.45              |
| 1:A:809:GLN:O     | 1:A:810:ASN:HB2   | 2.16                     | 0.45              |
| 1:A:892:GLU:O     | 1:A:899:VAL:HA    | 2.16                     | 0.45              |
| 1:B:6:VAL:HG22    | 1:B:1088:PHE:HD2  | 1.80                     | 0.45              |
| 1:B:23:PHE:N      | 1:B:30:ASN:ND2    | 2.53                     | 0.45              |
| 1:B:52:VAL:CG2    | 1:B:53:LYS:N      | 2.80                     | 0.45              |
| 1:B:1029:LEU:HD23 | 1:B:1039:LEU:HD13 | 1.97                     | 0.45              |
| 2:C:97:PRO:HA     | 2:C:202:ARG:HG2   | 1.97                     | 0.45              |
| 2:D:100:ASN:HB3   | 2:D:103:LEU:HD12  | 1.97                     | 0.45              |
| 1:A:130:MET:HE2   | 1:A:197:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:596:PHE:HB3   | 1:A:661:SER:HB2   | 1.98                     | 0.45              |
| 1:B:5:TYR:HE2     | 1:B:7:VAL:HG21    | 1.82                     | 0.45              |
| 1:B:250:PRO:O     | 1:B:252:ILE:N     | 2.49                     | 0.45              |
| 1:B:585:GLU:CD    | 1:B:585:GLU:N     | 2.74                     | 0.45              |
| 2:D:172:ARG:NH2   | 2:D:191:ASN:HD22  | 2.14                     | 0.45              |
| 1:A:166:ASP:HB3   | 1:A:219:VAL:HG23  | 1.98                     | 0.45              |
| 1:B:424:THR:HG22  | 1:B:425:LEU:N     | 2.32                     | 0.45              |
| 1:B:768:SER:C     | 1:B:769:LYS:HE2   | 2.41                     | 0.45              |
| 1:B:1110:ALA:C    | 1:B:1112:LEU:H    | 2.25                     | 0.45              |
| 2:C:35:THR:CG2    | 2:C:36:SER:O      | 2.33                     | 0.45              |
| 1:A:410:LEU:N     | 1:A:410:LEU:CD2   | 2.80                     | 0.45              |
| 1:A:864:LYS:HE2   | 1:A:891:TYR:CE2   | 2.49                     | 0.45              |
| 1:B:263:ARG:HB2   | 1:B:271:TYR:CE2   | 2.51                     | 0.45              |
| 1:B:539:ALA:HB2   | 1:B:561:TRP:CD1   | 2.51                     | 0.45              |
| 1:B:554:PRO:C     | 1:B:571:LEU:HB3   | 2.42                     | 0.45              |
| 1:B:690:SER:O     | 1:B:691:LEU:HD12  | 2.16                     | 0.45              |
| 1:B:853:TYR:HB2   | 1:B:858:LEU:HD23  | 1.99                     | 0.45              |
| 2:C:50:LEU:O      | 2:C:143:ARG:HB2   | 2.17                     | 0.45              |
| 1:A:520:GLN:HG3   | 1:A:529:ILE:CD1   | 2.47                     | 0.45              |
| 1:B:10:GLN:NE2    | 1:B:11:LYS:N      | 2.64                     | 0.45              |
| 1:B:196:SER:O     | 1:B:200:LYS:HA    | 2.16                     | 0.45              |
| 1:B:317:LEU:HD12  | 1:B:321:VAL:HG12  | 1.99                     | 0.45              |
| 1:B:402:ILE:HD13  | 1:B:699:LEU:HD12  | 1.99                     | 0.45              |
| 2:C:89:ASP:OD1    | 2:C:90:ASP:N      | 2.37                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:161:PHE:CE1  | 2:C:197:ILE:HG23  | 2.51                     | 0.45              |
| 2:D:109:PRO:HB2  | 2:D:203:ARG:HH21  | 1.81                     | 0.45              |
| 2:D:168:GLY:HA3  | 2:D:208:CYS:SG    | 2.55                     | 0.45              |
| 1:A:308:THR:O    | 1:A:383:LYS:NZ    | 2.49                     | 0.45              |
| 1:A:860:THR:HG22 | 1:A:860:THR:O     | 2.17                     | 0.45              |
| 1:B:29:LEU:HG    | 1:B:44:VAL:HG21   | 1.99                     | 0.45              |
| 1:B:397:HIS:O    | 1:B:702:GLY:HA3   | 2.16                     | 0.45              |
| 1:B:569:LEU:CD2  | 1:B:576:LEU:HA    | 2.46                     | 0.45              |
| 1:B:732:CYS:HB2  | 1:B:794:ILE:O     | 2.17                     | 0.45              |
| 1:B:1066:GLY:O   | 1:B:1067:LYS:HB2  | 2.16                     | 0.45              |
| 1:A:582:LEU:HD12 | 1:A:582:LEU:C     | 2.42                     | 0.45              |
| 1:A:584:GLY:O    | 1:B:900:ARG:NH2   | 2.49                     | 0.45              |
| 1:A:837:TYR:HB2  | 1:A:840:GLU:HG3   | 1.98                     | 0.45              |
| 1:B:63:VAL:CG2   | 1:B:80:LEU:HD23   | 2.47                     | 0.45              |
| 1:B:529:ILE:N    | 1:B:529:ILE:HD13  | 2.32                     | 0.45              |
| 1:B:644:LEU:HD23 | 1:B:645:SER:H     | 1.81                     | 0.45              |
| 2:D:17:ILE:HD11  | 2:D:139:ASN:HD22  | 1.80                     | 0.45              |
| 2:D:42:THR:HG22  | 2:D:43:ILE:N      | 2.31                     | 0.45              |
| 2:D:169:GLY:CA   | 2:D:211:CYS:HA    | 2.46                     | 0.45              |
| 1:B:42:TYR:CD2   | 1:B:49:LEU:HB3    | 2.52                     | 0.45              |
| 1:B:401:SER:C    | 1:B:402:ILE:HD12  | 2.41                     | 0.45              |
| 1:B:430:VAL:C    | 1:B:431:GLY:O     | 2.52                     | 0.45              |
| 1:B:451:PHE:HB2  | 1:B:486:LEU:HD13  | 1.98                     | 0.45              |
| 1:B:1127:ASP:HA  | 1:B:1130:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:16:ASN:CG    | 1:A:35:LYS:O      | 2.51                     | 0.44              |
| 1:A:304:LEU:HD12 | 1:A:305:LEU:H     | 1.82                     | 0.44              |
| 1:A:487:VAL:CG2  | 1:A:524:GLN:HA    | 2.46                     | 0.44              |
| 1:A:587:ILE:H    | 1:A:587:ILE:CD1   | 2.30                     | 0.44              |
| 1:B:37:THR:HG22  | 1:B:59:GLY:O      | 2.18                     | 0.44              |
| 1:B:63:VAL:HG21  | 1:B:80:LEU:HD23   | 1.98                     | 0.44              |
| 1:B:81:THR:OG1   | 1:B:85:ASN:HB2    | 2.16                     | 0.44              |
| 1:B:192:THR:CB   | 1:B:206:PRO:HD2   | 2.47                     | 0.44              |
| 1:B:392:ASN:ND2  | 1:B:392:ASN:C     | 2.75                     | 0.44              |
| 2:C:109:PRO:CG   | 2:C:203:ARG:NH1   | 2.80                     | 0.44              |
| 2:C:147:GLU:CG   | 2:C:172:ARG:HG3   | 2.47                     | 0.44              |
| 1:A:546:LEU:HD11 | 1:A:593:MET:HB3   | 1.99                     | 0.44              |
| 1:A:762:SER:HB3  | 1:A:803:HIS:ND1   | 2.32                     | 0.44              |
| 1:A:771:PHE:CD1  | 1:A:835:MET:HE2   | 2.52                     | 0.44              |
| 1:A:865:GLU:HG2  | 1:A:866:VAL:N     | 2.32                     | 0.44              |
| 1:B:139:LEU:HD22 | 1:B:156:ASN:HB3   | 1.99                     | 0.44              |
| 1:B:384:GLU:OE2  | 1:B:384:GLU:N     | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:894:THR:CG2  | 1:B:895:THR:N    | 2.78                     | 0.44              |
| 2:C:33:THR:HG22  | 2:C:35:THR:H     | 1.81                     | 0.44              |
| 2:C:98:ILE:HG13  | 2:C:189:TRP:CZ2  | 2.53                     | 0.44              |
| 1:A:518:TYR:C    | 1:A:518:TYR:CD2  | 2.95                     | 0.44              |
| 1:A:582:LEU:O    | 1:A:583:GLY:O    | 2.35                     | 0.44              |
| 1:A:808:LEU:HD12 | 1:A:835:MET:HE1  | 1.99                     | 0.44              |
| 1:B:10:GLN:HE21  | 1:B:11:LYS:N     | 2.16                     | 0.44              |
| 1:B:538:VAL:HG22 | 1:B:558:ILE:HD11 | 1.98                     | 0.44              |
| 2:D:116:ASP:O    | 2:D:182:ASP:CB   | 2.62                     | 0.44              |
| 1:A:282:MET:CG   | 1:A:305:LEU:HD11 | 2.44                     | 0.44              |
| 1:A:346:TYR:CD1  | 1:A:346:TYR:N    | 2.85                     | 0.44              |
| 1:B:573:SER:O    | 1:B:574:PHE:CB   | 2.66                     | 0.44              |
| 2:C:113:THR:HA   | 2:C:124:SER:O    | 2.17                     | 0.44              |
| 1:A:738:SER:OG   | 1:A:787:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:1121:LYS:HZ2 | 1:A:1121:LYS:HA  | 1.83                     | 0.44              |
| 1:B:124:ILE:HG12 | 1:B:131:ILE:HD12 | 1.99                     | 0.44              |
| 2:C:21:LEU:O     | 2:C:22:ASN:C     | 2.61                     | 0.44              |
| 2:C:103:LEU:O    | 2:C:104:GLY:C    | 2.61                     | 0.44              |
| 2:D:47:VAL:CG1   | 2:D:48:THR:N     | 2.80                     | 0.44              |
| 1:A:7:VAL:HG13   | 1:A:1091:GLY:HA3 | 2.00                     | 0.44              |
| 1:A:69:PRO:HD2   | 1:A:72:GLU:HG3   | 1.98                     | 0.44              |
| 1:A:874:VAL:HG13 | 1:A:881:LEU:HB3  | 2.00                     | 0.44              |
| 1:B:31:LEU:C     | 1:B:32:LEU:HD12  | 2.43                     | 0.44              |
| 1:B:704:ILE:H    | 1:B:704:ILE:CD1  | 2.29                     | 0.44              |
| 1:B:984:THR:O    | 1:B:986:ASP:N    | 2.51                     | 0.44              |
| 2:C:102:LEU:O    | 2:C:104:GLY:N    | 2.50                     | 0.44              |
| 1:A:704:ILE:HG23 | 1:A:705:ASP:N    | 2.32                     | 0.44              |
| 1:B:222:VAL:CG1  | 1:B:223:PRO:HD2  | 2.47                     | 0.44              |
| 1:B:342:GLU:O    | 1:B:344:GLY:N    | 2.51                     | 0.44              |
| 2:C:119:GLY:O    | 2:C:120:LYS:CB   | 2.66                     | 0.44              |
| 1:A:29:LEU:HG    | 1:A:44:VAL:CG2   | 2.47                     | 0.44              |
| 1:A:291:MET:HG3  | 1:A:292:ASP:N    | 2.29                     | 0.44              |
| 1:A:931:LEU:HD12 | 1:A:947:ARG:HH22 | 1.83                     | 0.44              |
| 1:B:47:GLU:HG2   | 1:B:48:GLY:N     | 2.25                     | 0.44              |
| 1:B:246:LEU:HD11 | 1:B:299:ASP:HA   | 1.99                     | 0.44              |
| 1:B:286:GLU:O    | 1:B:298:LYS:N    | 2.45                     | 0.44              |
| 1:B:416:ASP:HA   | 1:B:417:PRO:HD3  | 1.86                     | 0.44              |
| 1:B:482:GLU:HB2  | 1:B:483:PRO:CD   | 2.32                     | 0.44              |
| 1:B:482:GLU:CB   | 1:B:483:PRO:CD   | 2.92                     | 0.44              |
| 2:D:147:GLU:HA   | 2:D:148:PRO:HD3  | 1.83                     | 0.44              |
| 1:A:663:ASN:O    | 1:A:664:HIS:CB   | 2.64                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1007:PHE:CD2 | 1:A:1030:PHE:HB3  | 2.53                     | 0.44              |
| 1:B:140:PHE:CZ   | 1:B:178:ILE:HD12  | 2.53                     | 0.44              |
| 1:B:644:LEU:CG   | 1:B:645:SER:N     | 2.81                     | 0.44              |
| 1:B:1080:ARG:HG3 | 1:B:1081:LYS:N    | 2.32                     | 0.44              |
| 2:C:89:ASP:OD2   | 2:C:202:ARG:NH2   | 2.51                     | 0.44              |
| 2:C:102:LEU:C    | 2:C:104:GLY:N     | 2.75                     | 0.44              |
| 2:D:172:ARG:NE   | 2:D:174:GLU:OE2   | 2.50                     | 0.44              |
| 1:A:275:ASP:HB3  | 1:A:279:ARG:N     | 2.30                     | 0.43              |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:N     | 2.32                     | 0.43              |
| 1:B:376:VAL:HA   | 1:B:388:ARG:O     | 2.18                     | 0.43              |
| 1:B:616:LEU:HD12 | 1:B:617:ASN:H     | 1.80                     | 0.43              |
| 2:C:52:THR:HG21  | 2:C:85:ILE:HA     | 2.00                     | 0.43              |
| 1:A:1:MET:HA     | 1:A:1:MET:CE      | 2.48                     | 0.43              |
| 1:A:23:PHE:CE2   | 1:A:91:TYR:HB2    | 2.53                     | 0.43              |
| 1:A:78:PHE:O     | 1:A:79:ILE:HG12   | 2.18                     | 0.43              |
| 1:A:448:LEU:O    | 1:A:449:MET:C     | 2.60                     | 0.43              |
| 1:A:454:ASP:C    | 1:A:455:GLN:HG2   | 2.41                     | 0.43              |
| 1:A:480:SER:HB3  | 1:A:487:VAL:CG1   | 2.46                     | 0.43              |
| 1:A:705:ASP:OD2  | 1:A:709:LYS:CE    | 2.59                     | 0.43              |
| 1:A:734:GLY:HA3  | 1:A:829:PHE:CE1   | 2.53                     | 0.43              |
| 1:B:130:MET:HA   | 1:B:145:LEU:HB2   | 2.00                     | 0.43              |
| 1:B:192:THR:HB   | 1:B:206:PRO:HD2   | 2.00                     | 0.43              |
| 1:B:358:PRO:HA   | 1:B:1033:VAL:O    | 2.18                     | 0.43              |
| 1:B:1115:ASP:HB2 | 1:B:1120:MET:HB2  | 2.00                     | 0.43              |
| 1:A:90:GLU:HB3   | 1:A:101:ILE:HG13  | 2.00                     | 0.43              |
| 1:A:405:PRO:HA   | 1:A:697:SER:HA    | 2.00                     | 0.43              |
| 1:A:516:LEU:HD23 | 1:A:574:PHE:CE2   | 2.53                     | 0.43              |
| 1:B:9:ALA:HB3    | 1:B:1037:ILE:HG22 | 2.01                     | 0.43              |
| 1:B:81:THR:HG22  | 1:B:82:ALA:N      | 2.34                     | 0.43              |
| 1:B:261:HIS:ND1  | 1:B:261:HIS:C     | 2.76                     | 0.43              |
| 1:B:514:ARG:O    | 1:B:514:ARG:CG    | 2.63                     | 0.43              |
| 1:B:843:PRO:HG2  | 2:D:24:VAL:HG21   | 2.00                     | 0.43              |
| 2:D:148:PRO:O    | 2:D:149:ARG:C     | 2.61                     | 0.43              |
| 1:A:177:THR:HG22 | 1:A:194:GLU:HA    | 2.00                     | 0.43              |
| 1:A:744:ASP:HA   | 1:A:782:PHE:CE1   | 2.53                     | 0.43              |
| 1:A:936:LYS:HB3  | 1:A:939:GLU:HB2   | 2.00                     | 0.43              |
| 1:B:112:ILE:N    | 1:B:112:ILE:CD1   | 2.78                     | 0.43              |
| 1:B:150:LYS:HB2  | 1:B:151:GLU:OE2   | 2.18                     | 0.43              |
| 1:B:570:LYS:HE2  | 1:B:577:LEU:HD11  | 2.00                     | 0.43              |
| 1:B:694:ALA:HA   | 1:B:698:THR:O     | 2.18                     | 0.43              |
| 1:B:782:PHE:N    | 1:B:782:PHE:CD2   | 2.86                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1115:ASP:HA   | 1:B:1120:MET:HB3 | 2.00                     | 0.43              |
| 2:D:115:LEU:CD1   | 2:D:130:VAL:HG13 | 2.48                     | 0.43              |
| 1:A:679:MET:SD    | 1:A:680:CYS:N    | 2.92                     | 0.43              |
| 1:A:1032:THR:CG2  | 1:A:1034:ASN:H   | 2.23                     | 0.43              |
| 1:A:1039:LEU:HD12 | 1:A:1040:VAL:H   | 1.83                     | 0.43              |
| 1:B:263:ARG:HG2   | 1:B:263:ARG:HH11 | 1.83                     | 0.43              |
| 1:B:543:ILE:N     | 1:B:543:ILE:HD13 | 2.33                     | 0.43              |
| 1:B:874:VAL:HG22  | 1:B:875:GLU:O    | 2.18                     | 0.43              |
| 1:B:903:CYS:SG    | 1:B:941:ASN:HA   | 2.59                     | 0.43              |
| 2:D:211:CYS:HA    | 2:D:212:PRO:HD2  | 1.81                     | 0.43              |
| 1:A:762:SER:CB    | 1:A:803:HIS:ND1  | 2.82                     | 0.43              |
| 1:A:931:LEU:HD12  | 1:A:947:ARG:NH2  | 2.33                     | 0.43              |
| 1:B:222:VAL:HA    | 1:B:223:PRO:HD3  | 1.82                     | 0.43              |
| 1:B:237:ILE:HD11  | 1:B:253:ILE:HD11 | 2.00                     | 0.43              |
| 2:C:145:ILE:HD11  | 2:C:174:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:614:PHE:CD1   | 1:A:614:PHE:N    | 2.86                     | 0.43              |
| 1:B:248:ILE:O     | 1:B:250:PRO:HD3  | 2.19                     | 0.43              |
| 1:B:728:GLU:O     | 1:B:730:SER:N    | 2.51                     | 0.43              |
| 1:B:740:ILE:HD12  | 1:B:740:ILE:H    | 1.82                     | 0.43              |
| 1:B:832:GLY:N     | 1:B:873:MET:CE   | 2.82                     | 0.43              |
| 1:A:34:ALA:HB2    | 1:A:64:MET:HE1   | 2.00                     | 0.43              |
| 1:A:58:TYR:HB3    | 1:A:1073:TRP:HB2 | 2.01                     | 0.43              |
| 1:A:522:HIS:HB3   | 1:A:523:PRO:CD   | 2.49                     | 0.43              |
| 1:A:532:THR:CG2   | 1:A:533:GLU:N    | 2.81                     | 0.43              |
| 1:A:948:ASP:N     | 1:A:992:LEU:HD11 | 2.33                     | 0.43              |
| 1:B:45:THR:O      | 1:B:46:ALA:C     | 2.61                     | 0.43              |
| 1:B:155:PHE:HE1   | 1:B:157:ILE:HD11 | 1.83                     | 0.43              |
| 1:B:292:ASP:C     | 1:B:294:THR:H    | 2.27                     | 0.43              |
| 1:B:518:TYR:OH    | 1:B:571:LEU:HD11 | 2.18                     | 0.43              |
| 2:C:143:ARG:HH11  | 2:C:143:ARG:HG3  | 1.84                     | 0.43              |
| 2:D:80:ARG:HB2    | 2:D:81:PRO:CD    | 2.36                     | 0.43              |
| 1:A:10:GLN:HG2    | 1:A:710:LEU:HD12 | 1.99                     | 0.43              |
| 1:A:518:TYR:CE1   | 1:A:571:LEU:HD22 | 2.53                     | 0.43              |
| 1:B:170:LEU:HD11  | 1:B:179:CYS:HB2  | 2.00                     | 0.43              |
| 1:B:191:LYS:HD3   | 1:B:193:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:226:PHE:HB2   | 1:B:227:GLY:H    | 1.65                     | 0.43              |
| 1:B:281:PHE:O     | 1:B:305:LEU:HD12 | 2.18                     | 0.43              |
| 1:B:375:LEU:HD23  | 1:B:375:LEU:HA   | 1.85                     | 0.43              |
| 1:B:380:GLY:O     | 1:B:381:ALA:HB2  | 2.18                     | 0.43              |
| 1:B:452:VAL:HG22  | 1:B:453:ASP:N    | 2.34                     | 0.43              |
| 1:B:463:VAL:HG23  | 1:B:467:GLN:HB2  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:172:ARG:HH22  | 2:C:195:SER:C     | 2.27                     | 0.43              |
| 2:D:44:PRO:HA     | 2:D:45:PRO:HD3    | 1.94                     | 0.43              |
| 2:D:89:ASP:O      | 2:D:90:ASP:O      | 2.37                     | 0.43              |
| 2:D:192:PRO:CG    | 2:D:206:CYS:HB2   | 2.48                     | 0.43              |
| 2:D:218:CYS:CB    | 2:D:221:ASP:OD1   | 2.67                     | 0.43              |
| 1:A:295:VAL:HG23  | 1:A:295:VAL:O     | 2.18                     | 0.43              |
| 1:A:504:ASN:OD1   | 1:A:507:GLN:HG3   | 2.18                     | 0.43              |
| 1:A:946:ALA:HB2   | 1:A:989:ARG:O     | 2.19                     | 0.43              |
| 1:A:1032:THR:HG22 | 1:A:1035:GLY:N    | 2.34                     | 0.43              |
| 1:B:46:ALA:HB3    | 1:B:47:GLU:OE1    | 2.19                     | 0.43              |
| 1:B:194:GLU:OE2   | 1:B:204:LYS:O     | 2.36                     | 0.43              |
| 1:B:432:GLN:C     | 1:B:433:THR:OG1   | 2.61                     | 0.43              |
| 1:B:563:ASP:O     | 1:B:564:ILE:C     | 2.60                     | 0.43              |
| 1:B:894:THR:HG22  | 1:B:895:THR:H     | 1.82                     | 0.43              |
| 1:B:919:ASP:O     | 1:B:934:ALA:HA    | 2.19                     | 0.43              |
| 1:B:948:ASP:N     | 1:B:992:LEU:HD12  | 2.33                     | 0.43              |
| 1:B:1109:VAL:O    | 1:B:1110:ALA:O    | 2.37                     | 0.43              |
| 1:A:370:GLN:O     | 1:A:372:GLN:N     | 2.52                     | 0.42              |
| 1:A:391:ARG:HD2   | 1:A:392:ASN:O     | 2.19                     | 0.42              |
| 1:A:1097:PHE:CZ   | 1:A:1105:MET:CG   | 3.02                     | 0.42              |
| 1:B:183:GLN:HG2   | 1:B:184:ASP:N     | 2.34                     | 0.42              |
| 1:B:275:ASP:HB2   | 1:B:279:ARG:N     | 2.25                     | 0.42              |
| 1:B:355:ASN:O     | 1:B:357:GLY:N     | 2.52                     | 0.42              |
| 1:B:682:LEU:HD13  | 1:B:682:LEU:C     | 2.44                     | 0.42              |
| 1:B:843:PRO:HG2   | 2:D:24:VAL:CG2    | 2.49                     | 0.42              |
| 1:B:1108:VAL:HG12 | 1:B:1109:VAL:H    | 1.84                     | 0.42              |
| 2:C:38:LEU:O      | 2:C:39:GLY:C      | 2.60                     | 0.42              |
| 2:C:100:ASN:HB3   | 2:C:103:LEU:CG    | 2.49                     | 0.42              |
| 2:D:172:ARG:NH1   | 2:D:197:ILE:HG12  | 2.34                     | 0.42              |
| 2:D:173:ARG:HH12  | 2:D:218:CYS:CB    | 2.31                     | 0.42              |
| 1:A:403:ASP:HA    | 1:A:698:THR:HG22  | 2.02                     | 0.42              |
| 1:A:576:LEU:HD22  | 1:A:577:LEU:N     | 2.34                     | 0.42              |
| 1:A:745:THR:O     | 1:A:747:GLY:N     | 2.50                     | 0.42              |
| 1:A:912:LEU:HB2   | 1:A:913:TYR:CD1   | 2.54                     | 0.42              |
| 1:B:129:ARG:HH11  | 1:B:176:PRO:HD3   | 1.81                     | 0.42              |
| 1:B:161:GLU:N     | 1:B:161:GLU:CD    | 2.77                     | 0.42              |
| 1:B:1029:LEU:CD2  | 1:B:1039:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:127:GLU:O     | 1:A:128:CYS:HB2   | 2.20                     | 0.42              |
| 1:A:731:GLN:HA    | 1:A:796:GLN:NE2   | 2.34                     | 0.42              |
| 1:A:780:THR:HB    | 1:A:784:GLU:HG3   | 2.01                     | 0.42              |
| 1:B:181:VAL:HG23  | 1:B:219:VAL:CG2   | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:553:SER:HA    | 1:B:554:PRO:HD3   | 1.82                     | 0.42              |
| 1:B:655:ARG:NH1   | 1:B:655:ARG:HG2   | 2.35                     | 0.42              |
| 2:C:145:ILE:HA    | 2:C:145:ILE:HD13  | 1.74                     | 0.42              |
| 2:D:127:TYR:CE1   | 2:D:131:LYS:HD3   | 2.54                     | 0.42              |
| 1:A:570:LYS:HD2   | 1:A:570:LYS:HA    | 1.66                     | 0.42              |
| 1:A:660:TYR:CE2   | 1:A:708:GLN:OE1   | 2.72                     | 0.42              |
| 1:A:705:ASP:O     | 1:A:706:GLU:C     | 2.63                     | 0.42              |
| 1:A:866:VAL:HA    | 1:A:867:LYS:NZ    | 2.34                     | 0.42              |
| 1:A:970:ASN:OD1   | 1:A:970:ASN:C     | 2.62                     | 0.42              |
| 1:B:19:VAL:HG22   | 1:B:20:THR:N      | 2.33                     | 0.42              |
| 1:B:130:MET:HG2   | 1:B:197:LEU:HD11  | 2.01                     | 0.42              |
| 1:B:130:MET:HA    | 1:B:145:LEU:HB3   | 2.01                     | 0.42              |
| 1:B:1059:ASN:HD21 | 1:B:1070:HIS:CD2  | 2.36                     | 0.42              |
| 2:C:48:THR:HG22   | 2:C:83:ILE:O      | 2.18                     | 0.42              |
| 1:A:296:THR:OG1   | 1:A:297:LEU:N     | 2.53                     | 0.42              |
| 1:A:811:GLU:OE2   | 1:A:847:ARG:NE    | 2.53                     | 0.42              |
| 1:A:867:LYS:HD2   | 1:A:867:LYS:N     | 2.32                     | 0.42              |
| 1:A:1032:THR:HG23 | 1:A:1034:ASN:N    | 2.25                     | 0.42              |
| 1:B:235:GLU:HB2   | 1:B:254:LYS:HE3   | 2.00                     | 0.42              |
| 1:B:308:THR:OG1   | 1:B:324:VAL:HG11  | 2.19                     | 0.42              |
| 1:B:324:VAL:HB    | 1:B:332:GLN:HG2   | 2.02                     | 0.42              |
| 1:B:407:ILE:HG22  | 1:B:408:LYS:N     | 2.35                     | 0.42              |
| 1:B:414:ARG:NH2   | 1:B:462:ASN:HB2   | 2.34                     | 0.42              |
| 1:B:516:LEU:HD11  | 1:B:538:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:603:LEU:N     | 1:B:603:LEU:HD23  | 2.35                     | 0.42              |
| 1:B:662:SER:HB3   | 1:B:1138:ARG:HH21 | 1.85                     | 0.42              |
| 1:B:1030:PHE:O    | 1:B:1037:ILE:HA   | 2.19                     | 0.42              |
| 1:A:305:LEU:HD13  | 1:A:336:LEU:HD22  | 2.00                     | 0.42              |
| 1:A:549:SER:OG    | 1:A:550:ASN:N     | 2.53                     | 0.42              |
| 1:A:876:PHE:CD1   | 1:A:916:THR:HG21  | 2.55                     | 0.42              |
| 1:A:1053:ASP:O    | 1:A:1057:ARG:HG3  | 2.20                     | 0.42              |
| 1:B:130:MET:CE    | 1:B:195:VAL:HG11  | 2.50                     | 0.42              |
| 1:B:407:ILE:H     | 1:B:407:ILE:CD1   | 2.28                     | 0.42              |
| 1:B:458:PHE:HE2   | 1:B:499:SER:O     | 2.02                     | 0.42              |
| 1:B:818:SER:HA    | 1:B:828:TYR:O     | 2.19                     | 0.42              |
| 2:C:113:THR:HB    | 2:C:186:VAL:HB    | 2.00                     | 0.42              |
| 2:D:177:ILE:HG12  | 2:D:186:VAL:HG22  | 2.02                     | 0.42              |
| 1:A:910:MET:HG2   | 1:A:912:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:1000:LEU:HD13 | 1:A:1002:GLU:HB2  | 2.00                     | 0.42              |
| 1:B:162:LEU:HG    | 1:B:163:HIS:N     | 2.34                     | 0.42              |
| 1:B:182:TYR:CE1   | 1:B:189:HIS:HD2   | 2.38                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:412:PRO:HD3  | 1:B:680:CYS:HB2  | 2.02                     | 0.42              |
| 1:B:463:VAL:HG11 | 1:B:469:ILE:HB   | 2.01                     | 0.42              |
| 1:B:1017:LEU:C   | 1:B:1019:GLU:N   | 2.78                     | 0.42              |
| 1:B:388:ARG:C    | 1:B:389:ILE:HD12 | 2.45                     | 0.42              |
| 1:A:170:LEU:HD13 | 1:A:207:TRP:CH2  | 2.55                     | 0.42              |
| 1:A:854:SER:O    | 1:A:855:ASP:HB2  | 2.19                     | 0.42              |
| 1:A:1086:THR:C   | 1:A:1088:PHE:H   | 2.28                     | 0.42              |
| 1:B:4:ASN:ND2    | 1:B:976:VAL:HG11 | 2.34                     | 0.42              |
| 1:B:43:VAL:HG23  | 1:B:52:VAL:CG1   | 2.47                     | 0.42              |
| 1:B:394:ILE:HG13 | 1:B:669:SER:HB3  | 2.00                     | 0.42              |
| 1:B:467:GLN:CB   | 1:B:478:LEU:HD21 | 2.49                     | 0.42              |
| 1:B:724:ILE:HD11 | 1:B:733:PHE:CD2  | 2.54                     | 0.42              |
| 2:D:215:CYS:C    | 2:D:217:GLU:H    | 2.27                     | 0.42              |
| 1:A:177:THR:HG22 | 1:A:194:GLU:HG2  | 2.01                     | 0.42              |
| 1:A:964:ASN:OD1  | 1:A:978:GLN:HG3  | 2.20                     | 0.42              |
| 1:B:451:PHE:HD1  | 1:B:486:LEU:HD22 | 1.85                     | 0.42              |
| 1:B:915:LYS:HD3  | 1:B:915:LYS:HA   | 1.84                     | 0.42              |
| 2:D:22:ASN:O     | 2:D:25:GLU:N     | 2.50                     | 0.42              |
| 1:A:369:ARG:C    | 1:A:370:GLN:OE1  | 2.63                     | 0.41              |
| 1:A:550:ASN:C    | 1:A:552:LEU:H    | 2.27                     | 0.41              |
| 1:A:816:LEU:C    | 1:A:817:VAL:HG12 | 2.45                     | 0.41              |
| 1:B:235:GLU:O    | 1:B:236:SER:CB   | 2.68                     | 0.41              |
| 1:B:262:ASN:HD21 | 1:B:316:TYR:H    | 1.67                     | 0.41              |
| 1:B:381:ALA:O    | 1:B:382:PHE:HB2  | 2.20                     | 0.41              |
| 1:B:437:MET:HB2  | 1:B:446:THR:CG2  | 2.49                     | 0.41              |
| 1:B:503:CYS:HB2  | 1:B:508:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:613:TYR:CZ   | 1:B:627:LYS:HB2  | 2.55                     | 0.41              |
| 2:D:128:LYS:O    | 2:D:129:GLY:C    | 2.62                     | 0.41              |
| 1:A:173:CYS:C    | 1:A:175:ALA:N    | 2.76                     | 0.41              |
| 1:A:410:LEU:HA   | 1:A:426:VAL:O    | 2.20                     | 0.41              |
| 1:A:1113:GLN:CB  | 1:A:1121:LYS:HD2 | 2.49                     | 0.41              |
| 1:A:1114:TYR:CE2 | 1:A:1128:ASP:HB3 | 2.56                     | 0.41              |
| 1:B:63:VAL:O     | 1:B:79:ILE:HA    | 2.19                     | 0.41              |
| 1:B:130:MET:CG   | 1:B:197:LEU:HD11 | 2.51                     | 0.41              |
| 1:B:361:ASP:OD2  | 1:B:723:LYS:HD3  | 2.20                     | 0.41              |
| 1:B:396:ILE:CD1  | 1:B:673:LEU:HD11 | 2.42                     | 0.41              |
| 1:B:932:LEU:CD2  | 1:B:979:LYS:HD3  | 2.50                     | 0.41              |
| 1:B:1063:LYS:HG3 | 1:B:1063:LYS:O   | 2.20                     | 0.41              |
| 2:C:221:ASP:O    | 2:C:222:THR:HG23 | 2.20                     | 0.41              |
| 1:A:72:GLU:CD    | 1:A:103:ARG:HH22 | 2.29                     | 0.41              |
| 1:A:416:ASP:C    | 1:A:416:ASP:OD2  | 2.62                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:416:ASP:CG    | 1:A:419:ARG:HG3  | 2.44                     | 0.41              |
| 1:A:982:ALA:O     | 1:A:984:THR:N    | 2.50                     | 0.41              |
| 1:B:167:VAL:O     | 1:B:168:LYS:HE2  | 2.20                     | 0.41              |
| 1:B:250:PRO:C     | 1:B:252:ILE:N    | 2.78                     | 0.41              |
| 1:B:399:HIS:HB2   | 1:B:701:ILE:O    | 2.20                     | 0.41              |
| 1:B:910:MET:HE2   | 1:B:926:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:1058:LEU:HD23 | 1:B:1093:LEU:CD2 | 2.48                     | 0.41              |
| 1:B:1115:ASP:CB   | 1:B:1120:MET:HB2 | 2.50                     | 0.41              |
| 1:A:391:ARG:HB3   | 1:A:391:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:494:GLN:O     | 1:A:495:ALA:HB3  | 2.19                     | 0.41              |
| 1:A:597:GLU:HG3   | 1:A:661:SER:CB   | 2.50                     | 0.41              |
| 1:A:818:SER:O     | 1:A:819:CYS:HB3  | 2.20                     | 0.41              |
| 1:B:29:LEU:HD23   | 1:B:44:VAL:HG11  | 2.01                     | 0.41              |
| 1:B:582:LEU:HD12  | 1:B:582:LEU:C    | 2.46                     | 0.41              |
| 1:B:754:PRO:HB2   | 1:B:759:GLN:OE1  | 2.20                     | 0.41              |
| 2:C:111:THR:HB    | 2:C:188:GLU:CG   | 2.50                     | 0.41              |
| 2:C:112:GLN:HE22  | 2:C:187:THR:CG2  | 2.15                     | 0.41              |
| 2:C:170:PHE:HB2   | 2:C:193:SER:OG   | 2.20                     | 0.41              |
| 2:D:49:GLY:HA2    | 2:D:144:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:222:VAL:HA    | 1:A:223:PRO:HD3  | 1.83                     | 0.41              |
| 1:B:199:GLU:HG3   | 1:B:201:GLU:CD   | 2.46                     | 0.41              |
| 1:B:203:ASN:O     | 1:B:204:LYS:HB2  | 2.21                     | 0.41              |
| 1:B:483:PRO:O     | 1:B:484:LYS:CB   | 2.69                     | 0.41              |
| 1:B:644:LEU:H     | 1:B:644:LEU:CD2  | 2.32                     | 0.41              |
| 1:A:81:THR:HG21   | 1:A:85:ASN:OD1   | 2.21                     | 0.41              |
| 1:A:90:GLU:OE1    | 1:A:103:ARG:NE   | 2.53                     | 0.41              |
| 1:A:357:GLY:HA2   | 1:A:358:PRO:C    | 2.46                     | 0.41              |
| 1:A:362:MET:HB3   | 1:A:377:THR:HG22 | 2.03                     | 0.41              |
| 1:A:982:ALA:C     | 1:A:984:THR:N    | 2.77                     | 0.41              |
| 1:A:1013:VAL:HG12 | 1:A:1014:MET:O   | 2.21                     | 0.41              |
| 1:B:433:THR:OG1   | 1:B:455:GLN:O    | 2.24                     | 0.41              |
| 1:B:617:ASN:O     | 1:B:621:GLY:N    | 2.52                     | 0.41              |
| 2:C:216:SER:HA    | 2:C:219:GLU:CD   | 2.45                     | 0.41              |
| 2:D:113:THR:C     | 2:D:114:VAL:HG23 | 2.46                     | 0.41              |
| 2:D:147:GLU:OE2   | 2:D:163:ARG:CZ   | 2.69                     | 0.41              |
| 1:A:372:GLN:NE2   | 1:A:372:GLN:O    | 2.53                     | 0.41              |
| 1:A:388:ARG:CD    | 1:A:714:THR:HB   | 2.46                     | 0.41              |
| 1:B:459:PHE:HE2   | 1:B:503:CYS:SG   | 2.44                     | 0.41              |
| 1:B:1022:THR:O    | 1:B:1024:THR:N   | 2.54                     | 0.41              |
| 2:D:48:THR:HA     | 2:D:82:LYS:O     | 2.21                     | 0.41              |
| 1:A:7:VAL:HG11    | 1:A:1095:GLU:OE2 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:847:ARG:NH1  | 1:A:849:VAL:HG22  | 2.35                     | 0.41              |
| 1:B:383:LYS:CG   | 1:B:384:GLU:OE2   | 2.69                     | 0.41              |
| 1:B:473:SER:O    | 1:B:497:ASN:HA    | 2.21                     | 0.41              |
| 1:B:474:ALA:O    | 1:B:475:SER:CB    | 2.67                     | 0.41              |
| 1:B:886:SER:C    | 1:B:908:ASN:HD21  | 2.29                     | 0.41              |
| 2:C:215:CYS:SG   | 2:C:217:GLU:N     | 2.84                     | 0.41              |
| 1:A:16:ASN:HB2   | 1:A:35:LYS:O      | 2.21                     | 0.41              |
| 1:A:125:ASP:OD1  | 1:A:126:PRO:HD2   | 2.21                     | 0.41              |
| 1:A:181:VAL:HG23 | 1:A:219:VAL:CG2   | 2.50                     | 0.41              |
| 1:A:358:PRO:HD2  | 1:A:380:GLY:HA2   | 2.03                     | 0.41              |
| 1:A:622:LEU:HD23 | 1:A:622:LEU:H     | 1.86                     | 0.41              |
| 1:A:634:GLN:O    | 1:A:635:PRO:C     | 2.63                     | 0.41              |
| 1:A:725:CYS:SG   | 1:A:817:VAL:HA    | 2.60                     | 0.41              |
| 1:A:889:ARG:HD2  | 1:A:901:THR:CG2   | 2.51                     | 0.41              |
| 1:B:277:GLU:HB3  | 1:B:279:ARG:NH1   | 2.35                     | 0.41              |
| 1:B:287:LYS:HD3  | 1:B:287:LYS:O     | 2.20                     | 0.41              |
| 1:B:318:ASP:O    | 1:B:319:ASN:HB2   | 2.20                     | 0.41              |
| 1:B:408:LYS:HG3  | 1:B:430:VAL:HG23  | 2.03                     | 0.41              |
| 1:B:436:LEU:HD11 | 1:B:443:VAL:O     | 2.20                     | 0.41              |
| 1:B:724:ILE:HD11 | 1:B:733:PHE:HD2   | 1.86                     | 0.41              |
| 1:B:809:GLN:O    | 1:B:835:MET:HE1   | 2.21                     | 0.41              |
| 1:B:869:ALA:N    | 1:B:885:ASN:OD1   | 2.51                     | 0.41              |
| 1:B:933:LEU:HD23 | 1:B:944:GLU:HA    | 2.02                     | 0.41              |
| 1:B:1039:LEU:CD2 | 1:B:1139:ILE:HG22 | 2.50                     | 0.41              |
| 2:C:110:SER:N    | 2:C:221:ASP:HB3   | 2.35                     | 0.41              |
| 2:D:82:LYS:HE2   | 2:D:161:PHE:CZ    | 2.56                     | 0.41              |
| 1:A:18:CYS:HA    | 1:A:32:LEU:O      | 2.21                     | 0.41              |
| 1:A:224:GLU:O    | 1:A:225:PRO:C     | 2.63                     | 0.41              |
| 1:A:226:PHE:CD1  | 1:A:226:PHE:N     | 2.89                     | 0.41              |
| 1:A:537:GLU:HG3  | 1:A:561:TRP:CD1   | 2.56                     | 0.41              |
| 1:A:730:SER:HB2  | 1:A:732:CYS:SG    | 2.61                     | 0.41              |
| 1:A:841:ALA:HA   | 2:C:45:PRO:HG2    | 2.02                     | 0.41              |
| 1:B:450:GLY:CA   | 1:B:479:VAL:HG11  | 2.27                     | 0.41              |
| 1:B:570:LYS:C    | 1:B:572:PRO:HD2   | 2.46                     | 0.41              |
| 1:B:676:VAL:HG22 | 1:B:693:LEU:HD12  | 2.03                     | 0.41              |
| 1:B:836:VAL:HG13 | 2:D:22:ASN:OD1    | 2.21                     | 0.41              |
| 1:B:1108:VAL:C   | 1:B:1110:ALA:N    | 2.78                     | 0.41              |
| 2:C:147:GLU:OE2  | 2:C:163:ARG:HD3   | 2.21                     | 0.41              |
| 2:C:219:GLU:O    | 2:C:221:ASP:N     | 2.53                     | 0.41              |
| 2:D:142:THR:O    | 2:D:143:ARG:O     | 2.39                     | 0.41              |
| 1:A:90:GLU:HB3   | 1:A:101:ILE:CG1   | 2.51                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:439:ASN:O    | 1:A:440:GLY:C     | 2.65                     | 0.40              |
| 1:A:676:VAL:HG11 | 1:A:693:LEU:HD22  | 2.03                     | 0.40              |
| 1:B:5:TYR:CE2    | 1:B:7:VAL:HG21    | 2.56                     | 0.40              |
| 1:B:213:GLU:OE1  | 1:B:234:GLN:O     | 2.38                     | 0.40              |
| 1:B:456:GLN:O    | 1:B:472:THR:HB    | 2.21                     | 0.40              |
| 1:B:706:GLU:OE1  | 1:B:706:GLU:C     | 2.65                     | 0.40              |
| 1:A:22:HIS:CD2   | 1:A:28:ASP:O      | 2.74                     | 0.40              |
| 1:A:125:ASP:HA   | 1:A:126:PRO:HD3   | 1.97                     | 0.40              |
| 1:A:1109:VAL:O   | 1:A:1109:VAL:HG12 | 2.22                     | 0.40              |
| 1:B:991:HIS:HB3  | 1:B:993:GLN:HE22  | 1.86                     | 0.40              |
| 1:B:994:GLU:O    | 1:B:995:VAL:CG2   | 2.60                     | 0.40              |
| 2:C:107:SER:O    | 2:C:109:PRO:HD2   | 2.21                     | 0.40              |
| 1:A:263:ARG:HD2  | 1:A:265:ASP:O     | 2.22                     | 0.40              |
| 1:A:439:ASN:O    | 1:A:442:GLU:N     | 2.47                     | 0.40              |
| 1:A:439:ASN:O    | 1:A:441:GLU:N     | 2.55                     | 0.40              |
| 1:A:542:ASP:HB3  | 1:A:557:ALA:HB3   | 2.03                     | 0.40              |
| 1:B:2:SER:CB     | 1:B:995:VAL:HG23  | 2.51                     | 0.40              |
| 1:B:254:LYS:HD2  | 1:B:254:LYS:N     | 2.36                     | 0.40              |
| 1:B:740:ILE:HG22 | 1:B:741:GLU:N     | 2.36                     | 0.40              |
| 1:B:949:PHE:CE1  | 1:B:991:HIS:CD2   | 3.10                     | 0.40              |
| 1:B:1061:VAL:O   | 1:B:1062:ILE:C    | 2.64                     | 0.40              |
| 1:A:484:LYS:O    | 1:A:485:ALA:HB2   | 2.22                     | 0.40              |
| 1:A:568:ILE:O    | 1:A:569:LEU:HD23  | 2.20                     | 0.40              |
| 1:A:607:GLY:HA2  | 1:A:635:PRO:HA    | 2.04                     | 0.40              |
| 1:B:284:LEU:CD1  | 1:B:301:ARG:NH2   | 2.84                     | 0.40              |
| 2:C:52:THR:HG21  | 2:C:85:ILE:CA     | 2.50                     | 0.40              |
| 1:A:166:ASP:O    | 1:A:180:PHE:HB2   | 2.21                     | 0.40              |
| 1:A:234:GLN:O    | 1:A:235:GLU:HG2   | 2.20                     | 0.40              |
| 1:A:471:ILE:HG23 | 1:A:476:VAL:HB    | 2.04                     | 0.40              |
| 1:A:492:GLU:OE2  | 1:A:494:GLN:N     | 2.54                     | 0.40              |
| 1:A:611:LEU:C    | 1:A:611:LEU:CD2   | 2.89                     | 0.40              |
| 1:A:837:TYR:HA   | 1:A:838:PRO:HD3   | 1.95                     | 0.40              |
| 1:B:281:PHE:HB3  | 1:B:282:MET:H     | 1.67                     | 0.40              |
| 1:B:378:CYS:SG   | 1:B:724:ILE:HB    | 2.60                     | 0.40              |
| 1:B:447:GLU:C    | 1:B:448:LEU:HD12  | 2.46                     | 0.40              |
| 1:B:507:GLN:NE2  | 1:B:552:LEU:HA    | 2.37                     | 0.40              |
| 1:B:569:LEU:HD23 | 1:B:576:LEU:HA    | 2.03                     | 0.40              |
| 1:B:1047:TRP:O   | 1:B:1048:TYR:C    | 2.62                     | 0.40              |
| 1:B:1120:MET:HB2 | 1:B:1121:LYS:H    | 1.72                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 1126/1140 (99%) | 960 (85%)  | 128 (11%) | 38 (3%)  | 3           | 6 |
| 1   | B     | 1130/1140 (99%) | 892 (79%)  | 145 (13%) | 93 (8%)  | 0           | 1 |
| 2   | C     | 168/222 (76%)   | 123 (73%)  | 33 (20%)  | 12 (7%)  | 1           | 1 |
| 2   | D     | 169/222 (76%)   | 115 (68%)  | 32 (19%)  | 22 (13%) | 0           | 0 |
| All | All   | 2593/2724 (95%) | 2090 (81%) | 338 (13%) | 165 (6%) | 1           | 1 |

All (165) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 254 | LYS  |
| 1   | A     | 269 | SER  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 341 | ASN  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 371 | GLY  |
| 1   | A     | 708 | GLN  |
| 1   | A     | 772 | SER  |
| 1   | A     | 781 | SER  |
| 1   | A     | 856 | GLY  |
| 1   | A     | 929 | SER  |
| 1   | B     | 46  | ALA  |
| 1   | B     | 223 | PRO  |
| 1   | B     | 275 | ASP  |
| 1   | B     | 310 | ILE  |
| 1   | B     | 341 | ASN  |
| 1   | B     | 357 | GLY  |
| 1   | B     | 430 | VAL  |
| 1   | B     | 434 | ARG  |
| 1   | B     | 450 | GLY  |
| 1   | B     | 466 | GLN  |
| 1   | B     | 493 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 549  | SER  |
| 1   | B     | 551  | GLY  |
| 1   | B     | 576  | LEU  |
| 1   | B     | 688  | PRO  |
| 1   | B     | 707  | ILE  |
| 1   | B     | 751  | ALA  |
| 1   | B     | 782  | PHE  |
| 1   | B     | 985  | THR  |
| 1   | B     | 1015 | GLN  |
| 1   | B     | 1016 | ASN  |
| 1   | B     | 1021 | SER  |
| 1   | B     | 1065 | VAL  |
| 1   | B     | 1109 | VAL  |
| 1   | B     | 1110 | ALA  |
| 2   | C     | 39   | GLY  |
| 2   | C     | 108  | THR  |
| 2   | C     | 162  | LYS  |
| 2   | D     | 23   | THR  |
| 2   | D     | 51   | LEU  |
| 2   | D     | 89   | ASP  |
| 2   | D     | 90   | ASP  |
| 2   | D     | 104  | GLY  |
| 2   | D     | 108  | THR  |
| 2   | D     | 109  | PRO  |
| 2   | D     | 143  | ARG  |
| 2   | D     | 193  | SER  |
| 2   | D     | 209  | HIS  |
| 1   | A     | 118  | THR  |
| 1   | A     | 147  | ARG  |
| 1   | A     | 203  | ASN  |
| 1   | A     | 294  | THR  |
| 1   | A     | 449  | MET  |
| 1   | A     | 524  | GLN  |
| 1   | A     | 551  | GLY  |
| 1   | A     | 583  | GLY  |
| 1   | A     | 643  | SER  |
| 1   | A     | 646  | THR  |
| 1   | A     | 706  | GLU  |
| 1   | A     | 746  | SER  |
| 1   | A     | 983  | ALA  |
| 1   | A     | 987  | GLU  |
| 1   | B     | 26   | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 35   | LYS  |
| 1   | B     | 113  | GLY  |
| 1   | B     | 146  | ASP  |
| 1   | B     | 149  | ASN  |
| 1   | B     | 168  | LYS  |
| 1   | B     | 214  | ALA  |
| 1   | B     | 276  | MET  |
| 1   | B     | 318  | ASP  |
| 1   | B     | 369  | ARG  |
| 1   | B     | 451  | PHE  |
| 1   | B     | 524  | GLN  |
| 1   | B     | 564  | ILE  |
| 1   | B     | 626  | ARG  |
| 1   | B     | 729  | VAL  |
| 1   | B     | 748  | GLY  |
| 1   | B     | 986  | ASP  |
| 1   | B     | 995  | VAL  |
| 1   | B     | 1037 | ILE  |
| 1   | B     | 1066 | GLY  |
| 1   | B     | 1119 | GLY  |
| 2   | C     | 148  | PRO  |
| 2   | C     | 180  | VAL  |
| 2   | C     | 220  | ARG  |
| 2   | D     | 105  | LEU  |
| 2   | D     | 148  | PRO  |
| 2   | D     | 149  | ARG  |
| 2   | D     | 216  | SER  |
| 1   | A     | 367  | LEU  |
| 1   | A     | 368  | GLU  |
| 1   | A     | 817  | VAL  |
| 1   | A     | 1015 | GLN  |
| 1   | A     | 1027 | SER  |
| 1   | B     | 147  | ARG  |
| 1   | B     | 148  | ASP  |
| 1   | B     | 236  | SER  |
| 1   | B     | 343  | GLN  |
| 1   | B     | 432  | GLN  |
| 1   | B     | 433  | THR  |
| 1   | B     | 440  | GLY  |
| 1   | B     | 444  | GLU  |
| 1   | B     | 465  | HIS  |
| 1   | B     | 475  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 484  | LYS  |
| 1   | B     | 578  | HIS  |
| 1   | B     | 884  | ILE  |
| 1   | B     | 1080 | ARG  |
| 2   | C     | 103  | LEU  |
| 2   | C     | 107  | SER  |
| 2   | D     | 39   | GLY  |
| 2   | D     | 91   | LYS  |
| 2   | D     | 117  | LEU  |
| 1   | A     | 319  | ASN  |
| 1   | B     | 226  | PHE  |
| 1   | B     | 251  | PRO  |
| 1   | B     | 253  | ILE  |
| 1   | B     | 255  | GLN  |
| 1   | B     | 340  | SER  |
| 1   | B     | 706  | GLU  |
| 1   | B     | 761  | LEU  |
| 1   | B     | 783  | GLY  |
| 1   | B     | 864  | LYS  |
| 1   | B     | 918  | GLY  |
| 1   | B     | 984  | THR  |
| 2   | C     | 50   | LEU  |
| 2   | D     | 19   | THR  |
| 2   | D     | 99   | PRO  |
| 1   | A     | 184  | ASP  |
| 1   | A     | 224  | GLU  |
| 1   | A     | 440  | GLY  |
| 1   | A     | 937  | PRO  |
| 1   | B     | 47   | GLU  |
| 1   | B     | 203  | ASN  |
| 1   | B     | 208  | LYS  |
| 1   | B     | 241  | ASN  |
| 1   | B     | 243  | ASP  |
| 1   | B     | 356  | LEU  |
| 1   | B     | 381  | ALA  |
| 1   | B     | 572  | PRO  |
| 1   | B     | 575  | GLU  |
| 1   | B     | 643  | SER  |
| 1   | B     | 861  | VAL  |
| 1   | B     | 1036 | MET  |
| 2   | C     | 195  | SER  |
| 2   | D     | 212  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 253  | ILE  |
| 1   | B     | 204  | LYS  |
| 1   | B     | 486  | LEU  |
| 1   | B     | 1111 | ASN  |
| 2   | D     | 192  | PRO  |
| 1   | A     | 584  | GLY  |
| 1   | B     | 513  | GLY  |
| 1   | B     | 822  | GLY  |
| 2   | C     | 164  | GLY  |
| 2   | D     | 180  | VAL  |
| 1   | B     | 571  | LEU  |
| 1   | B     | 1013 | VAL  |
| 2   | C     | 20   | GLY  |
| 1   | A     | 119  | GLY  |
| 1   | B     | 144  | PRO  |
| 1   | B     | 224  | GLU  |
| 1   | B     | 848  | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 992/999 (99%)   | 897 (90%)  | 95 (10%) | 8           | 17 |
| 1   | B     | 994/999 (100%)  | 916 (92%)  | 78 (8%)  | 11          | 25 |
| 2   | C     | 151/191 (79%)   | 130 (86%)  | 21 (14%) | 3           | 6  |
| 2   | D     | 151/191 (79%)   | 133 (88%)  | 18 (12%) | 5           | 10 |
| All | All   | 2288/2380 (96%) | 2076 (91%) | 212 (9%) | 8           | 18 |

All (212) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 6   | VAL  |
| 1   | A     | 7   | VAL  |
| 1   | A     | 10  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | GLU  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 52  | VAL  |
| 1   | A     | 68  | ARG  |
| 1   | A     | 79  | ILE  |
| 1   | A     | 81  | THR  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 112 | ILE  |
| 1   | A     | 117 | GLU  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 147 | ARG  |
| 1   | A     | 167 | VAL  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 186 | GLN  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 206 | PRO  |
| 1   | A     | 235 | GLU  |
| 1   | A     | 282 | MET  |
| 1   | A     | 291 | MET  |
| 1   | A     | 297 | LEU  |
| 1   | A     | 298 | LYS  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 312 | GLU  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 391 | ARG  |
| 1   | A     | 392 | ASN  |
| 1   | A     | 396 | ILE  |
| 1   | A     | 410 | LEU  |
| 1   | A     | 414 | ARG  |
| 1   | A     | 449 | MET  |
| 1   | A     | 455 | GLN  |
| 1   | A     | 468 | LEU  |
| 1   | A     | 476 | VAL  |
| 1   | A     | 481 | GLN  |
| 1   | A     | 487 | VAL  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 525 | GLU  |
| 1   | A     | 531 | HIS  |
| 1   | A     | 552 | LEU  |
| 1   | A     | 567 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 571  | LEU  |
| 1   | A     | 576  | LEU  |
| 1   | A     | 579  | LYS  |
| 1   | A     | 587  | ILE  |
| 1   | A     | 589  | ARG  |
| 1   | A     | 594  | THR  |
| 1   | A     | 599  | SER  |
| 1   | A     | 624  | SER  |
| 1   | A     | 647  | THR  |
| 1   | A     | 648  | ASN  |
| 1   | A     | 682  | LEU  |
| 1   | A     | 696  | ASN  |
| 1   | A     | 700  | THR  |
| 1   | A     | 704  | ILE  |
| 1   | A     | 705  | ASP  |
| 1   | A     | 708  | GLN  |
| 1   | A     | 713  | ARG  |
| 1   | A     | 714  | THR  |
| 1   | A     | 759  | GLN  |
| 1   | A     | 765  | VAL  |
| 1   | A     | 781  | SER  |
| 1   | A     | 791  | LEU  |
| 1   | A     | 796  | GLN  |
| 1   | A     | 817  | VAL  |
| 1   | A     | 823  | LYS  |
| 1   | A     | 835  | MET  |
| 1   | A     | 839  | GLU  |
| 1   | A     | 858  | LEU  |
| 1   | A     | 866  | VAL  |
| 1   | A     | 867  | LYS  |
| 1   | A     | 874  | VAL  |
| 1   | A     | 884  | ILE  |
| 1   | A     | 902  | GLU  |
| 1   | A     | 907  | ASN  |
| 1   | A     | 925  | ASP  |
| 1   | A     | 931  | LEU  |
| 1   | A     | 957  | VAL  |
| 1   | A     | 966  | LEU  |
| 1   | A     | 969  | GLU  |
| 1   | A     | 990  | GLN  |
| 1   | A     | 992  | LEU  |
| 1   | A     | 1000 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1032 | THR  |
| 1   | A     | 1041 | THR  |
| 1   | A     | 1062 | ILE  |
| 1   | A     | 1069 | GLU  |
| 1   | A     | 1093 | LEU  |
| 1   | A     | 1121 | LYS  |
| 1   | A     | 1135 | GLU  |
| 1   | B     | 6    | VAL  |
| 1   | B     | 24   | THR  |
| 1   | B     | 35   | LYS  |
| 1   | B     | 53   | LYS  |
| 1   | B     | 92   | LYS  |
| 1   | B     | 109  | GLN  |
| 1   | B     | 112  | ILE  |
| 1   | B     | 130  | MET  |
| 1   | B     | 162  | LEU  |
| 1   | B     | 185  | PRO  |
| 1   | B     | 255  | GLN  |
| 1   | B     | 275  | ASP  |
| 1   | B     | 277  | GLU  |
| 1   | B     | 287  | LYS  |
| 1   | B     | 302  | VAL  |
| 1   | B     | 304  | LEU  |
| 1   | B     | 307  | GLU  |
| 1   | B     | 312  | GLU  |
| 1   | B     | 354  | THR  |
| 1   | B     | 367  | LEU  |
| 1   | B     | 392  | ASN  |
| 1   | B     | 402  | ILE  |
| 1   | B     | 427  | LEU  |
| 1   | B     | 449  | MET  |
| 1   | B     | 456  | GLN  |
| 1   | B     | 466  | GLN  |
| 1   | B     | 477  | ARG  |
| 1   | B     | 481  | GLN  |
| 1   | B     | 493  | PRO  |
| 1   | B     | 498  | ILE  |
| 1   | B     | 524  | GLN  |
| 1   | B     | 529  | ILE  |
| 1   | B     | 543  | ILE  |
| 1   | B     | 567  | ARG  |
| 1   | B     | 581  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 585  | GLU  |
| 1   | B     | 597  | GLU  |
| 1   | B     | 603  | LEU  |
| 1   | B     | 614  | PHE  |
| 1   | B     | 630  | THR  |
| 1   | B     | 699  | LEU  |
| 1   | B     | 704  | ILE  |
| 1   | B     | 706  | GLU  |
| 1   | B     | 713  | ARG  |
| 1   | B     | 746  | SER  |
| 1   | B     | 749  | THR  |
| 1   | B     | 750  | THR  |
| 1   | B     | 769  | LYS  |
| 1   | B     | 780  | THR  |
| 1   | B     | 781  | SER  |
| 1   | B     | 790  | ASN  |
| 1   | B     | 793  | ILE  |
| 1   | B     | 815  | SER  |
| 1   | B     | 839  | GLU  |
| 1   | B     | 852  | GLN  |
| 1   | B     | 866  | VAL  |
| 1   | B     | 885  | ASN  |
| 1   | B     | 899  | VAL  |
| 1   | B     | 901  | THR  |
| 1   | B     | 908  | ASN  |
| 1   | B     | 931  | LEU  |
| 1   | B     | 941  | ASN  |
| 1   | B     | 943  | GLU  |
| 1   | B     | 957  | VAL  |
| 1   | B     | 969  | GLU  |
| 1   | B     | 980  | ASP  |
| 1   | B     | 995  | VAL  |
| 1   | B     | 1000 | LEU  |
| 1   | B     | 1036 | MET  |
| 1   | B     | 1040 | VAL  |
| 1   | B     | 1043 | LEU  |
| 1   | B     | 1052 | LEU  |
| 1   | B     | 1078 | THR  |
| 1   | B     | 1086 | THR  |
| 1   | B     | 1093 | LEU  |
| 1   | B     | 1120 | MET  |
| 1   | B     | 1131 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1134 | GLU  |
| 2   | C     | 37   | SER  |
| 2   | C     | 50   | LEU  |
| 2   | C     | 106  | ASP  |
| 2   | C     | 108  | THR  |
| 2   | C     | 111  | THR  |
| 2   | C     | 114  | VAL  |
| 2   | C     | 121  | THR  |
| 2   | C     | 137  | LYS  |
| 2   | C     | 145  | ILE  |
| 2   | C     | 163  | ARG  |
| 2   | C     | 176  | SER  |
| 2   | C     | 179  | TRP  |
| 2   | C     | 190  | CYS  |
| 2   | C     | 194  | CYS  |
| 2   | C     | 197  | ILE  |
| 2   | C     | 206  | CYS  |
| 2   | C     | 208  | CYS  |
| 2   | C     | 210  | GLN  |
| 2   | C     | 211  | CYS  |
| 2   | C     | 218  | CYS  |
| 2   | C     | 222  | THR  |
| 2   | D     | 17   | ILE  |
| 2   | D     | 18   | GLU  |
| 2   | D     | 25   | GLU  |
| 2   | D     | 51   | LEU  |
| 2   | D     | 86   | VAL  |
| 2   | D     | 101  | PRO  |
| 2   | D     | 102  | LEU  |
| 2   | D     | 111  | THR  |
| 2   | D     | 122  | LEU  |
| 2   | D     | 140  | LEU  |
| 2   | D     | 143  | ARG  |
| 2   | D     | 145  | ILE  |
| 2   | D     | 163  | ARG  |
| 2   | D     | 192  | PRO  |
| 2   | D     | 194  | CYS  |
| 2   | D     | 208  | CYS  |
| 2   | D     | 213  | VAL  |
| 2   | D     | 215  | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4    | ASN  |
| 1   | A     | 22   | HIS  |
| 1   | A     | 30   | ASN  |
| 1   | A     | 156  | ASN  |
| 1   | A     | 186  | GLN  |
| 1   | A     | 234  | GLN  |
| 1   | A     | 241  | ASN  |
| 1   | A     | 262  | ASN  |
| 1   | A     | 290  | GLN  |
| 1   | A     | 319  | ASN  |
| 1   | A     | 341  | ASN  |
| 1   | A     | 343  | GLN  |
| 1   | A     | 372  | GLN  |
| 1   | A     | 374  | GLN  |
| 1   | A     | 455  | GLN  |
| 1   | A     | 467  | GLN  |
| 1   | A     | 481  | GLN  |
| 1   | A     | 507  | GLN  |
| 1   | A     | 520  | GLN  |
| 1   | A     | 522  | HIS  |
| 1   | A     | 578  | HIS  |
| 1   | A     | 648  | ASN  |
| 1   | A     | 672  | ASN  |
| 1   | A     | 711  | HIS  |
| 1   | A     | 790  | ASN  |
| 1   | A     | 796  | GLN  |
| 1   | A     | 809  | GLN  |
| 1   | A     | 810  | ASN  |
| 1   | A     | 904  | ASN  |
| 1   | A     | 907  | ASN  |
| 1   | A     | 990  | GLN  |
| 1   | A     | 991  | HIS  |
| 1   | A     | 1016 | ASN  |
| 1   | A     | 1034 | ASN  |
| 1   | A     | 1055 | GLN  |
| 1   | A     | 1056 | ASN  |
| 1   | A     | 1070 | HIS  |
| 1   | A     | 1140 | HIS  |
| 1   | B     | 4    | ASN  |
| 1   | B     | 22   | HIS  |
| 1   | B     | 30   | ASN  |
| 1   | B     | 105  | HIS  |
| 1   | B     | 109  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 189  | HIS  |
| 1   | B     | 203  | ASN  |
| 1   | B     | 209  | GLN  |
| 1   | B     | 255  | GLN  |
| 1   | B     | 262  | ASN  |
| 1   | B     | 267  | ASN  |
| 1   | B     | 290  | GLN  |
| 1   | B     | 343  | GLN  |
| 1   | B     | 372  | GLN  |
| 1   | B     | 392  | ASN  |
| 1   | B     | 397  | HIS  |
| 1   | B     | 399  | HIS  |
| 1   | B     | 456  | GLN  |
| 1   | B     | 466  | GLN  |
| 1   | B     | 481  | GLN  |
| 1   | B     | 497  | ASN  |
| 1   | B     | 507  | GLN  |
| 1   | B     | 524  | GLN  |
| 1   | B     | 711  | HIS  |
| 1   | B     | 743  | GLN  |
| 1   | B     | 790  | ASN  |
| 1   | B     | 796  | GLN  |
| 1   | B     | 803  | HIS  |
| 1   | B     | 826  | ASN  |
| 1   | B     | 877  | ASN  |
| 1   | B     | 904  | ASN  |
| 1   | B     | 941  | ASN  |
| 1   | B     | 973  | ASN  |
| 1   | B     | 991  | HIS  |
| 1   | B     | 993  | GLN  |
| 1   | B     | 1015 | GLN  |
| 1   | B     | 1034 | ASN  |
| 1   | B     | 1070 | HIS  |
| 1   | B     | 1140 | HIS  |
| 2   | C     | 30   | GLN  |
| 2   | C     | 112  | GLN  |
| 2   | C     | 210  | GLN  |
| 2   | D     | 22   | ASN  |
| 2   | D     | 30   | GLN  |
| 2   | D     | 31   | GLN  |
| 2   | D     | 41   | ASN  |
| 2   | D     | 100  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 112 | GLN  |
| 2   | D     | 191 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | D     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 189:TRP   | C      | 190:CYS   | N      | 0.99         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 1132/1140 (99%) | -0.05  | 25 (2%) 62 53  | 18, 47, 99, 160       | 0     |
| 1   | B     | 1134/1140 (99%) | 0.39   | 47 (4%) 41 32  | 29, 68, 122, 173      | 0     |
| 2   | C     | 174/222 (78%)   | 0.66   | 21 (12%) 8 6   | 32, 62, 118, 183      | 0     |
| 2   | D     | 175/222 (78%)   | 1.05   | 31 (17%) 4 3   | 39, 81, 138, 168      | 0     |
| All | All   | 2615/2724 (95%) | 0.26   | 124 (4%) 36 28 | 18, 59, 117, 183      | 0     |

All (124) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 453  | ASP  | 5.4  |
| 1   | B     | 571  | LEU  | 4.7  |
| 2   | D     | 20   | GLY  | 4.6  |
| 1   | A     | 708  | GLN  | 4.6  |
| 2   | D     | 16   | LEU  | 4.4  |
| 1   | B     | 1018 | GLY  | 4.2  |
| 1   | B     | 162  | LEU  | 4.1  |
| 2   | D     | 15   | LYS  | 4.1  |
| 1   | B     | 750  | THR  | 4.1  |
| 1   | B     | 367  | LEU  | 4.0  |
| 2   | D     | 165  | ARG  | 3.9  |
| 2   | C     | 161  | PHE  | 3.8  |
| 1   | B     | 464  | ALA  | 3.8  |
| 2   | C     | 164  | GLY  | 3.8  |
| 2   | C     | 218  | CYS  | 3.6  |
| 1   | B     | 981  | SER  | 3.6  |
| 1   | B     | 746  | SER  | 3.6  |
| 2   | C     | 152  | PRO  | 3.5  |
| 1   | A     | 644  | LEU  | 3.5  |
| 1   | A     | 571  | LEU  | 3.4  |
| 1   | A     | 706  | GLU  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1119 | GLY  | 3.3  |
| 1   | B     | 456  | GLN  | 3.2  |
| 1   | A     | 924  | GLY  | 3.2  |
| 1   | B     | 368  | GLU  | 3.2  |
| 2   | D     | 163  | ARG  | 3.2  |
| 2   | C     | 165  | ARG  | 3.1  |
| 1   | B     | 206  | PRO  | 3.1  |
| 1   | A     | 783  | GLY  | 3.1  |
| 1   | A     | 884  | ILE  | 3.1  |
| 2   | C     | 206  | CYS  | 3.0  |
| 1   | B     | 748  | GLY  | 3.0  |
| 1   | B     | 448  | LEU  | 3.0  |
| 2   | D     | 209  | HIS  | 3.0  |
| 2   | D     | 148  | PRO  | 3.0  |
| 1   | B     | 452  | VAL  | 3.0  |
| 2   | C     | 50   | LEU  | 2.9  |
| 2   | D     | 102  | LEU  | 2.9  |
| 2   | D     | 215  | CYS  | 2.9  |
| 2   | D     | 92   | THR  | 2.9  |
| 2   | D     | 169  | GLY  | 2.9  |
| 1   | B     | 1015 | GLN  | 2.9  |
| 2   | D     | 218  | CYS  | 2.9  |
| 2   | C     | 151  | ASN  | 2.7  |
| 1   | B     | 980  | ASP  | 2.7  |
| 1   | B     | 455  | GLN  | 2.7  |
| 1   | B     | 451  | PHE  | 2.7  |
| 2   | C     | 16   | LEU  | 2.7  |
| 2   | D     | 208  | CYS  | 2.7  |
| 2   | D     | 198  | THR  | 2.7  |
| 1   | B     | 443  | VAL  | 2.7  |
| 1   | B     | 844  | LYS  | 2.6  |
| 2   | D     | 83   | ILE  | 2.6  |
| 2   | D     | 161  | PHE  | 2.6  |
| 2   | C     | 180  | VAL  | 2.6  |
| 2   | C     | 162  | LYS  | 2.6  |
| 2   | D     | 104  | GLY  | 2.6  |
| 2   | C     | 52   | THR  | 2.6  |
| 1   | A     | 983  | ALA  | 2.6  |
| 2   | D     | 26   | TYR  | 2.5  |
| 1   | A     | 707  | ILE  | 2.5  |
| 1   | B     | 369  | ARG  | 2.5  |
| 1   | A     | 1016 | ASN  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 140  | LEU  | 2.5  |
| 2   | D     | 38   | LEU  | 2.5  |
| 1   | B     | 643  | SER  | 2.5  |
| 2   | D     | 214  | THR  | 2.4  |
| 1   | B     | 1017 | LEU  | 2.4  |
| 2   | D     | 107  | SER  | 2.4  |
| 2   | D     | 21   | LEU  | 2.4  |
| 2   | C     | 53   | ASN  | 2.4  |
| 1   | A     | 709  | LYS  | 2.4  |
| 1   | B     | 178  | ILE  | 2.4  |
| 2   | D     | 159  | ILE  | 2.4  |
| 1   | B     | 430  | VAL  | 2.4  |
| 1   | A     | 1022 | THR  | 2.4  |
| 1   | B     | 422  | TYR  | 2.4  |
| 1   | B     | 449  | MET  | 2.4  |
| 1   | B     | 984  | THR  | 2.4  |
| 2   | C     | 211  | CYS  | 2.3  |
| 2   | C     | 38   | LEU  | 2.3  |
| 2   | D     | 166  | ASP  | 2.3  |
| 2   | C     | 208  | CYS  | 2.3  |
| 1   | A     | 1017 | LEU  | 2.3  |
| 1   | A     | 857  | LYS  | 2.3  |
| 2   | D     | 33   | THR  | 2.3  |
| 2   | D     | 101  | PRO  | 2.3  |
| 1   | B     | 1    | MET  | 2.3  |
| 1   | A     | 759  | GLN  | 2.3  |
| 1   | B     | 857  | LYS  | 2.3  |
| 2   | C     | 215  | CYS  | 2.3  |
| 1   | B     | 646  | THR  | 2.2  |
| 1   | B     | 450  | GLY  | 2.2  |
| 1   | A     | 761  | LEU  | 2.2  |
| 1   | A     | 548  | ASP  | 2.2  |
| 2   | D     | 108  | THR  | 2.2  |
| 1   | A     | 662  | SER  | 2.2  |
| 1   | B     | 1014 | MET  | 2.2  |
| 1   | B     | 707  | ILE  | 2.2  |
| 1   | A     | 1018 | GLY  | 2.2  |
| 1   | B     | 300  | LEU  | 2.2  |
| 1   | B     | 225  | PRO  | 2.1  |
| 1   | B     | 218  | MET  | 2.1  |
| 2   | D     | 105  | LEU  | 2.1  |
| 1   | A     | 981  | SER  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 413 | LEU  | 2.1  |
| 1   | B     | 207 | TRP  | 2.1  |
| 1   | B     | 247 | ALA  | 2.1  |
| 1   | A     | 210 | GLU  | 2.1  |
| 1   | B     | 190 | VAL  | 2.1  |
| 2   | D     | 17  | ILE  | 2.1  |
| 2   | C     | 108 | THR  | 2.1  |
| 1   | A     | 207 | TRP  | 2.1  |
| 2   | D     | 103 | LEU  | 2.0  |
| 1   | A     | 111 | ARG  | 2.0  |
| 1   | A     | 918 | GLY  | 2.0  |
| 1   | A     | 449 | MET  | 2.0  |
| 1   | B     | 852 | GLN  | 2.0  |
| 1   | B     | 405 | PRO  | 2.0  |
| 2   | D     | 190 | CYS  | 2.0  |
| 2   | C     | 117 | LEU  | 2.0  |
| 1   | B     | 884 | ILE  | 2.0  |
| 1   | B     | 780 | THR  | 2.0  |
| 2   | C     | 33  | THR  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | ZN   | C     | 3001 | 1/1   | 0.89 | 0.13 | 35,35,35,35                 | 0     |
| 3   | ZN   | C     | 3002 | 1/1   | 0.90 | 0.11 | 35,35,35,35                 | 0     |
| 3   | ZN   | D     | 3004 | 1/1   | 0.95 | 0.18 | 35,35,35,35                 | 0     |
| 3   | ZN   | D     | 3003 | 1/1   | 0.98 | 0.15 | 35,35,35,35                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.